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Orthogonal Polynomials

Computation and Approximation

WALTER GAUTSCHI

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Orthogonal Polynomials
Computation and Approximation

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CONTENTS

PREFACE

The main purpose of this book is to present an account of computational methods for generating orthogonal polynomials on the real line (or part thereof), to discuss a number of related applications, and to provide software necessary for implementing all methods and applications.

The choice of topics, admittedly, is influenced by the author's own past involvement in this area, but it is hoped that the treatment given, and especially the software provided, will be useful to a large segment of the readership.

In Chapter 1, a brief, but essentially self-contained, review of the theory of orthogonal polynomials is presented, which emphasizes those parts of the theory that are most relevant to computation. The computational methods themselves are treated in Chapter 2. They are basically of two kinds, those based on moment information and those based on discretization. Other miscellaneous methods also receive attention, such as the computation of Cauchy integrals, modification algorithms for the underlying measures, and computing orthogonal polynomials of Sobolev type. Chapter 3 is devoted to applications, specifically numerical quadrature, discrete least squares approximation, moment-preserving spline approximation, and the summation of slowly convergent series. Historical comments and references to related topics not treated in this book are given in separate Notes to each chapter.

All software are in the form of Matlab scripts, which are collected in a suite of Matlab programs called `OPQ`, and which are downloadable individually from the Web Site

`http://www.cs.purdue.edu/archives/2002/wxg/codes/`

Occasionally, there will be a need to refer to a quadruple-precision version `ORTHPOLq` of the Fortran package in Gautschi (1994). This can be found on the Web Site

`http://www.cs.purdue.edu/archives/2001/wxg/codes/`

Many tables throughout the book report on numerical results of various algorithms. All numbers in these tables are displayed in floating-point format $m(e)$, where m, $1 \le m < 10$, is the mantissa of the number, and e the signed exponent.

The author is grateful to Gene H. Golub for his encouragement to write this book. He also acknowledges helpful comments by Olav Njåstad and Lothar Reichel.

I dedicate this book to my wife, Erika, in appreciation of her patience and unwavering support.

December, 2003 Walter Gautschi

To
Erika

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1

BASIC THEORY

This introductory chapter is to present a quick review of material on orthogonal polynomials that is particularly relevant to computation. Proofs of most results are included; for those requiring more extensive analytic treatments, references are made to the literature.

1.1 Orthogonal polynomials

1.1.1 *Definition and existence*

Let $\lambda(t)$ be a nondecreasing function on the real line $\mathbb{R}$ having finite limits as $t \to -\infty$ and $t \to +\infty$, and assume that the induced positive measure $\mathrm{d}\lambda$ has finite moments of all orders,

$$\mu_r = \mu_r(\mathrm{d}\lambda) := \int_{\mathbb{R}} t^r \,\mathrm{d}\lambda(t), \quad r = 0, 1, 2, \ldots, \quad \text{with } \mu_0 > 0. \tag{1.1.1}$$

Let $\mathbb{P}$ be the space of real polynomials and $\mathbb{P}_d \subset \mathbb{P}$ the space of polynomials of degree $\leq d$. For any pair u, v in $\mathbb{P}$, one may define an *inner product* as

$$(u, v) = \int_{\mathbb{R}} u(t)v(t) \,\mathrm{d}\lambda(t). \tag{1.1.2}$$

If $(u, v) = 0$, then u is said to be *orthogonal* to v. If $u = v$, then

$$\|u\| = \sqrt{(u, u)} = \left(\int_{\mathbb{R}} u^2(t) \,\mathrm{d}\lambda(t) \right)^{1/2} \tag{1.1.3}$$

is called the *norm* of u. (We write $(u, v)_{\mathrm{d}\lambda}$ and $\|u\|_{\mathrm{d}\lambda}$ if we want to exhibit the measure $\mathrm{d}\lambda$.) Clearly, $\|u\| \geq 0$ for all $u \in \mathbb{P}$. *Schwarz's inequality* states that

$$|(u, v)| \leq \|u\| \, \|v\|. \tag{1.1.4}$$

Definition 1.1 *The inner product (1.1.2) is said to be* positive definite *on* $\mathbb{P}$ *if* $\|u\| > 0$ *for all* $u \in \mathbb{P}$, $u \not\equiv 0$. *It is said to be positive definite on* $\mathbb{P}_d$ *if* $\|u\| > 0$ *for any* $u \in \mathbb{P}_d$, $u \not\equiv 0$.

Hankel determinants in the moments μ_r,

$$\Delta_n = \det \boldsymbol{M}_n, \qquad \boldsymbol{M}_n = \begin{bmatrix} \mu_0 & \mu_1 & \cdots & \mu_{n-1} \\ \mu_1 & \mu_2 & \cdots & \mu_n \\ \vdots & \vdots & & \vdots \\ \mu_{n-1} & \mu_n & \cdots & \mu_{2n-2} \end{bmatrix}, \quad n = 1, 2, 3, \ldots, \tag{1.1.5}$$

provide a simple criterion for positive definiteness.

Theorem 1.2 *The inner product (1.1.2) is positive definite on* $\mathbb{P}$ *if and only if*

$$\Delta_n > 0, \quad n = 1, 2, 3, \dots \ . \tag{1.1.6}$$

It is positive definite on $\mathbb{P}_d$ *if and only if* $\Delta_n > 0$ *for* $n = 1, 2, \dots, d+1$.

Proof Consider first the space $\mathbb{P}_d$, and let $u \in \mathbb{P}_d$, $u = c_0 + c_1 t + \cdots + c_d t^d$. Since

$$\|u\|^2 = \int_{\mathbb{R}} \sum_{k,\ell=0}^{d} c_k c_\ell t^{k+\ell} \, \mathrm{d}\lambda(t) = \sum_{k,\ell=0}^{d} \mu_{k+\ell} c_k c_\ell, \tag{1.1.7}$$

positive definiteness on $\mathbb{P}_d$ is equivalent to the Hankel matrix $\boldsymbol{M}_{d+1}$ being positive definite. This, in turn, is equivalent to $\Delta_n > 0$ for $n = 1, 2, \dots, d+1$. The case $d = \infty$ gives the result for $\mathbb{P}$. □

Definition 1.3 *Monic real polynomials* $\pi_k(t) = t^k + \cdots$, $k = 0, 1, 2, \dots$, *are called* monic orthogonal polynomials with respect to the measure $\mathrm{d}\lambda$, *and will be denoted by* $\pi_k(\,\cdot\,) = \pi_k(\,\cdot\,; \mathrm{d}\lambda)$, *if*

$$\begin{gathered} (\pi_k, \pi_\ell)_{\mathrm{d}\lambda} = 0 \quad \textit{for } k \neq \ell, \quad k, l = 0, 1, 2, \dots \ \textit{and} \\ \|\pi_k\|_{\mathrm{d}\lambda} > 0 \quad \textit{for } k = 0, 1, 2, \dots \ . \end{gathered} \tag{1.1.8}$$

There are infinitely many orthogonal polynomials if the index set $k = 0, 1, 2, \dots$ *is unbounded, and finitely many otherwise.* Normalization $\tilde{\pi}_k = \pi_k / \|\pi_k\|$, $k = 0, 1, 2, \dots$, *yields the* orthonormal polynomials, *which satisfy*

$$(\tilde{\pi}_k, \tilde{\pi}_\ell)_{\mathrm{d}\lambda} = \delta_{k\ell} := \begin{cases} 0 & \text{if } k \neq \ell, \\ 1 & \text{if } k = \ell. \end{cases} \tag{1.1.9}$$

They will be denoted by $\tilde{\pi}_k(\,\cdot\,) = \tilde{\pi}_k(\,\cdot\,; \mathrm{d}\lambda)$.

Lemma 1.4 *Let* π_k, $k = 0, 1, \dots, n$, *be monic orthogonal polynomials. If* $p \in \mathbb{P}_n$ *satisfies* $(p, \pi_k) = 0$ *for* $k = 0, 1, \dots, n$, *then* $p \equiv 0$.

Proof Writing $p(t) = a_0 + a_1 t + \cdots + a_n t^n$, one has

$$0 = (p, \pi_n) = a_n (t^n, \pi_n) = a_n (\pi_n, \pi_n).$$

Since $(\pi_n, \pi_n) > 0$, this yields $a_n = 0$. Similarly, one shows, in turn, that $a_{n-1} = 0$, $a_{n-2} = 0, \dots, a_0 = 0$. □

Lemma 1.5 *A set* $\pi_0, \pi_1, \dots, \pi_n$ *of monic orthogonal polynomials is linearly independent. Moreover, any polynomial* $p \in \mathbb{P}_n$ *can be uniquely represented in the form*

$$p = \sum_{k=0}^{n} c_k \pi_k \tag{1.1.10}$$

for some real constants c_k. *In other words,* $\pi_0, \pi_1, \dots, \pi_n$ *forms a* basis *of* $\mathbb{P}_n$.

Proof If $\sum_{k=0}^{n} \gamma_k \pi_k \equiv 0$, taking the inner product of both sides with π_j, $j = 0, 1, \ldots, n$, yields by orthogonality $\gamma_j = 0$. This proves linear independence. Writing p in the form (1.1.10) and taking the inner product of both sides with π_j gives $c_j = (p, \pi_j)/(\pi_j, \pi_j)$, $j = 0, 1, \ldots, n$. With the coefficients c_k so defined, $p - \sum_{k=0}^{n} c_k \pi_k$ is orthogonal to $\pi_0, \pi_1, \ldots, \pi_n$, hence, by Lemma 1.4, identically zero. □

Theorem 1.6 *If the inner product (1.1.2) is positive definite on $\mathbb{P}$, there exists a unique infinite sequence $\{\pi_k\}$ of monic orthogonal polynomials.*

Proof The polynomials π_k can be generated by applying *Gram–Schmidt orthogonalization* to the sequence of powers, $e_k(t) = t^k$, $k = 0, 1, 2, \ldots$. Thus, one takes $\pi_0 = 1$ and for $k = 1, 2, 3, \ldots$ recursively generates

$$\pi_k = e_k - \sum_{\ell=0}^{k-1} c_\ell \pi_\ell, \quad c_\ell = \frac{(e_k, \pi_\ell)}{(\pi_\ell, \pi_\ell)}. \tag{1.1.11}$$

Since $(\pi_\ell, \pi_\ell) > 0$ by the positive definiteness of the inner product, the polynomial π_k is uniquely defined and, by construction, is orthogonal to all polynomials π_j, $j < k$. □

The hypothesis of Theorem 1.6 is satisfied if λ has infinitely many points of increase, that is, points t_0 such that $\lambda(t_0 + \varepsilon) - \lambda(t_0 - \varepsilon) > 0$ for all $\varepsilon > 0$. The set of all points of increase of λ is called the *support* (or *spectrum*) of the measure $\mathrm{d}\lambda$ and its convex hull the *support interval* of $\mathrm{d}\lambda$.

Theorem 1.7 *If the inner product (1.1.2) is positive definite on $\mathbb{P}_d$ but not on $\mathbb{P}_n$ for any $n > d$, there exists only a finite number $d+1$ of orthogonal polynomials $\pi_0, \pi_1, \ldots, \pi_d$.*

Proof The Gram–Schmidt procedure (1.1.11) can be applied as long as the denominators (π_ℓ, π_ℓ) in the formula for c_ℓ remain positive, that is, for $k \le d+1$. The last polynomial π_{d+1} so constructed is orthogonal to all π_j, $j \le d$, where $\pi_0, \pi_1, \ldots, \pi_d$ are mutually orthogonal and of positive norm. However, π_{d+1} has norm zero. Indeed, by assumption there exists a monic polynomial $\omega \in \mathbb{P}_{d+1}$ such that $\|\omega\| = 0$. Since $\omega - \pi_{d+1}$ has degree d, by Lemma 1.5 there holds

$$\omega = \pi_{d+1} + \sum_{j=0}^{d} \gamma_j \pi_j$$

for certain coefficients γ_j. Consequently,

$$0 = \|\omega\|^2 = \|\pi_{d+1}\|^2 + \sum_{j=0}^{d} \gamma_j^2 \|\pi_j\|^2,$$

which implies $\|\pi_{d+1}\| = 0$. Thus, π_{d+1} cannot be a member of a sequence of orthogonal polynomials. □

Theorem 1.8 *If the moments (1.1.1) of* $\mathrm{d}\lambda$ *exist only for* $r = 0, 1, \ldots, r_0$*, there exists only a finite number* $d+1$ *of orthogonal polynomials* $\pi_0, \pi_1, \ldots, \pi_d$*, where* $d = \lfloor r_0/2 \rfloor$.

Proof The Gram–Schmidt procedure (1.1.11) can be carried out as long as the inner products in (1.1.11), including (π_k, π_k), exist, that is, for $2k \le r_0$ or, for what is the same, $k \le d$. □

Many of the measures occurring in applications are *absolutely continuous* whereby $\mathrm{d}\lambda(t) = w(t)\,\mathrm{d}t$ and w is a nonnegative integrable function on $\mathbb{R}$ called the *weight function*. The corresponding orthogonal and orthonormal polynomials will be denoted also by $\pi_k(\,\cdot\,; w)$ resp. $\tilde{\pi}_k(\,\cdot\,; w)$. The support of $\mathrm{d}\lambda$ is normally an interval—finite, half-infinite, or infinite—or possibly a finite number of disjoint intervals. A *discrete measure* $\mathrm{d}\lambda$ is one whose support consists of a finite or denumerably infinite number of distinct points t_k at which λ has positive jumps w_k. If the number of points is finite and equal to N, the discrete measure will be denoted by $\mathrm{d}\lambda_N$. The inner product associated with it is

$$\int_{\mathbb{R}} u(t)v(t)\,\mathrm{d}\lambda_N(t) = \sum_{k=1}^{N} w_k u(t_k)v(t_k). \tag{1.1.12}$$

It is positive definite on $\mathbb{P}_{N-1}$, but not on any $\mathbb{P}_n$ with $n \ge N$. By Theorem 1.7, there exist only N orthogonal polynomials $\pi_0, \pi_1, \ldots, \pi_{N-1}$. They are called *discrete orthogonal polynomials* and satisfy

$$\sum_{k=1}^{N} w_k \pi_r(t_k)\pi_s(t_k) = \|\pi_r\|^2 \delta_{rs}. \tag{1.1.13}$$

Theorem 1.9 *Let* $\pi_0, \pi_1, \ldots, \pi_{N-1}$ *be the monic orthogonal polynomials relative to the discrete measure* $\mathrm{d}\lambda_N$ *of (1.1.12). Then, they satisfy not only (1.1.13), but also*

$$\sum_{k=0}^{N-1} \frac{1}{\|\pi_k\|^2}\,\pi_k(t_r)\pi_k(t_s) = \frac{1}{w_r}\,\delta_{rs}. \tag{1.1.14}$$

Proof The orthogonality condition (1.1.13) can be written in matrix form as $\boldsymbol{Q}^{\mathrm{T}}\boldsymbol{Q} = \boldsymbol{I}$, where $\boldsymbol{Q} \in \mathbb{R}^{N\times N}$ is the matrix with elements $q_{rs} = \pi_s(t_r)\sqrt{w_r}/\|\pi_s\|$. Then also $\boldsymbol{Q}\boldsymbol{Q}^{\mathrm{T}} = \boldsymbol{I}$, which is precisely (1.1.14). □

Orthogonality in the sense of (1.1.14) is referred to as *dual orthogonality*.

1.1.2 *Examples*

Examples of measures that are sufficiently unconventional to require numerical techniques for the generation of the corresponding orthogonal polynomials, but are of interest in applications, will now be presented. The phrase "$\mathrm{d}\lambda(t)$ on $[a, b]$" will be used as a shorthand expression for "the support of $\mathrm{d}\lambda$ is the interval $[a, b]$"; thus, $\mathrm{d}\lambda(t) \equiv 0$ for t outside of $[a, b]$.

Example 1.10 $\mathrm{d}\lambda(t) = t^\alpha \ln(1/t)\,\mathrm{d}t$ on $[0,1]$, $\alpha > -1$.

All moments μ_r of $\mathrm{d}\lambda$ are finite, in fact, equal to $(r+\alpha+1)^{-1}$, and the inner product (1.1.2) is positive definite on $\mathbb{P}$. The corresponding orthogonal polynomials are useful to construct Gaussian quadrature rules (cf. §3.1.1) for integrals over $[0,1]$ whose integrands have two singularities at the origin, one logarithmic and the other algebraic (if α is not a nonnegative integer); see Example 2.27 of §2.1.9.

Example 1.11 $\mathrm{d}\lambda(t) = \mathrm{e}^{-t}\,\mathrm{d}t$ and $\mathrm{d}\lambda(t) = \mathrm{e}^{-t^2}\,\mathrm{d}t$ on $[0,c]$, $0 < c < \infty$.

These are Laguerre resp. Hermite measures (cf. §1.5.1) on a finite interval. Their moments are expressible in terms of the incomplete gamma function $\gamma(\alpha,x) = \int_0^x t^{\alpha-1}\mathrm{e}^{-t}\,\mathrm{d}t$ as $\mu_r = \gamma(r+1,c)$ resp. $\mu_r = \frac{1}{2}\gamma(\frac{1}{2}(r-1),c^2)$. Both measures are useful in Gaussian integration of integrals commonly encountered in molecular quantum mechanics. The underlying orthogonal polynomials go under the name *Mach polynomials* (Mach, 1984) in the former, and *Rys polynomials* (King and Dupuis, 1976) in the latter case. See also Steen, Byrne, and Gelbard (1969) and Chin (1992).

Example 1.12 $\mathrm{d}\lambda(t) = w(t)\,\mathrm{d}t$ where

$$w(t) = \begin{cases} |t|^\gamma (t^2-\xi^2)^\alpha (1-t^2)^\beta & \text{if } t \in (-1,-\xi)\cup(\xi,1), \\ 0 & \text{otherwise} \end{cases} \tag{1.1.15}$$

and $0 < \xi < 1$, $\alpha > -1$, $\beta > -1$, $\gamma \in \mathbb{R}$.

This is an example of a (symmetric) measure supported on two disjoint intervals $[-1,-\xi]$ and $[\xi,1]$. The respective orthogonal polynomials are studied in Barkov (1960), also in the more general (asymmetric) case where $|t|$ in eqn (1.1.15) is replaced by $|t+c|$. The special case $\gamma = 1$, $\alpha = \beta = -\frac{1}{2}$, $\xi = (1-\rho)/(1+\rho)$ $(0 < \rho < 1)$ arises in the study of the diatomic linear chain (Wheeler, 1984, where the basic support interval extends from 0 to 1 rather than from –1 to 1). The quantity ρ in this context has the meaning of a mass ratio $\rho = m/M$, where m and M $(m < M)$ are the masses of the two kinds of particles alternating along the chain. See also Example 2.30 in §2.1.9.

Example 1.13 $\mathrm{d}\lambda(t) = t^\alpha \mathrm{e}^{-t^2}\,\mathrm{d}t$ on $[0,\infty]$, $\alpha > -1$.

The moments of $\mathrm{d}\lambda$ are $\mu_r = \Gamma(\frac{1}{2}(r+\alpha+1))$ and the inner product (1.1.2) is positive definite on $\mathbb{P}$. For $\alpha = 2$ the measure is identical with the Maxwell velocity distribution in the kinetic theory of gases. The corresponding orthogonal polynomials are, therefore, referred to as *Maxwell polynomials* or *speed polynomials*. They have found application in the numerical solution of the Boltzmann equation by a discrete ordinate method (Shizgal, 1981) and also in the calculation of the eigenvalues of the Lorentz Fokker–Planck equation (Shizgal, 1979). The case $\alpha = 0$, referred to as the *half-range Hermite measure* (cf. Example 2.31 in §2.1.9), occurs in the calculation of effective radiative neutron capture cross-sections in nuclear reactor design (Steen, Byrne, and Gelbard, 1969). It also has statistical applications (Kahaner, Tietjen, and Beckman, 1982).

Example 1.14 $\mathrm{d}\lambda(t) = t^2\left(1+t^2/\omega\right)^{-\omega-1}\,\mathrm{d}t$ on $[0,\infty]$, $\omega > 1$.

In this example, the moment μ_r exists only if $r < 2\omega-1$, so that in Theorem 1.8 one has $r_0 = 2\omega-2$ if ω is an integer, and $r_0 = \lfloor 2\omega-1\rfloor$ otherwise. Accordingly, there exist only $d+1$ orthogonal polynomials, where $d = \omega-1$ resp. $d = \lfloor \omega - \frac{1}{2}\rfloor$. As $\omega \to \infty$, they tend to the Maxwell polynomials of Example 1.13. For finite ω they are useful in the study of space plasma, where Lorentzian rather than Maxwellian velocity distributions are often observed. They have been named, therefore, *Lorentzian polynomials* (Pierrard and Magnus, 2003).

The final example is a discrete measure supported on N distinct points. It is neither unconventional nor in need of numerical techniques. The corresponding discrete orthogonal polynomials indeed have been used already by Chebyshev (1859) in connection with discrete least squares approximation (cf. §3.2.1). See also Table 1.2.

Example 1.15 $\mathrm{d}\lambda_N(x) = \sum_{k=0}^{N-1}\delta(x-k)\,\mathrm{d}x$, δ = Dirac delta function.

Thus, $\mathrm{d}\lambda_N$ is supported on the N equally spaced points $0,1,2,\ldots,N-1$ and has unit jumps there. The corresponding orthogonal polynomials are, up to a constant factor,

$$t_n(x) = n!\,\Delta^n\left\{\binom{x}{n}\binom{x-N}{n}\right\}, \quad n = 0,1,2,\ldots,N-1, \tag{1.1.16}$$

where Δ is the forward difference operator with unit spacing acting on the variable x; cf. Szegö (1975, eqn (2.8.1)). See also Examples 2.26 and 2.35.

1.2 Properties of orthogonal polynomials

We assume in this section that $\mathrm{d}\lambda$ is a positive measure on $\mathbb{R}$ with infinitely many points of increase unless stated otherwise, and with finite moments (1.1.1) of all orders.

1.2.1 *Symmetry*

Definition 1.16 *An absolutely continuous measure* $\mathrm{d}\lambda(t) = w(t)\,\mathrm{d}t$ *is* symmetric *(with respect to the origin) if its support interval is* $[-a,a]$, $0 < a \le \infty$, *and* $w(-t) = w(t)$ *for all* $t \in \mathbb{R}$. *A discrete measure* $\mathrm{d}\lambda_N = \sum_{k=1}^{N} w_k\delta(t-t_k)\,\mathrm{d}t$ *is symmetric if* $t_k = -t_{N+1-k}$, $w_k = w_{N+1-k}$ *for* $k = 1,2,\ldots,N$.

Theorem 1.17 *If* $\mathrm{d}\lambda$ *is symmetric, then*

$$\pi_k(-t;\mathrm{d}\lambda) = (-1)^k\pi_k(t;\mathrm{d}\lambda), \quad k = 0,1,2,\ldots\ . \tag{1.2.1}$$

Thus, π_k *is an even or odd polynomial depending on the parity of* k.

Proof Define $\hat{\pi}_k(t) = (-1)^k\pi_k(-t;\mathrm{d}\lambda)$. One computes

$$(\hat{\pi}_k,\hat{\pi}_\ell)_{\mathrm{d}\lambda} = (-1)^{k+\ell}(\pi_k,\pi_\ell)_{\mathrm{d}\lambda} = 0 \quad \text{if } k \ne \ell.$$

Since all $\hat{\pi}_k$ are monic, $\hat{\pi}_k(t) \equiv \pi_k(t;\mathrm{d}\lambda)$ by the uniqueness of monic orthogonal polynomials. □

Theorem 1.18 *Let* $\mathrm{d}\lambda$ *be symmetric on* $[-a,a]$, $0<a\le\infty$, *and*

$$\pi_{2k}(t;\mathrm{d}\lambda)=\pi_k^+(t^2),\quad \pi_{2k+1}(t;\mathrm{d}\lambda)=t\pi_k^-(t^2). \tag{1.2.2}$$

Then $\{\pi_k^\pm\}$ *are the monic orthogonal polynomials with respect to the measure* $\mathrm{d}\lambda^\pm(t)=t^{\mp 1/2}w(t^{1/2})\,\mathrm{d}t$ *on* $[0,a^2]$.

Proof We prove the assertion for π_k^+; the proof for π_k^- is analogous.

Clearly, π_k^+ is monic. By symmetry, $0=(\pi_{2k},\pi_{2\ell})_{\mathrm{d}\lambda}=2\int_0^a \pi_{2k}(t)\pi_{2\ell}(t)w(t)\,\mathrm{d}t$ if $k\ne\ell$; hence, by the first of (1.2.2),

$$0=2\int_0^a \pi_k^+(t^2)\pi_\ell^+(t^2)w(t)\,\mathrm{d}t=\int_0^{a^2}\pi_k^+(\tau)\pi_\ell^+(\tau)\tau^{-1/2}w(\tau^{1/2})\,\mathrm{d}\tau,\quad k\ne\ell.$$

□

1.2.2 *Zeros*

Theorem 1.19 *All zeros of* $\pi_n(\,\cdot\,)=\pi_n(\,\cdot\,;\mathrm{d}\lambda)$, $n\ge 1$, *are real, simple, and located in the interior of the support interval* $[a,b]$ *of* $\mathrm{d}\lambda$.

Proof Since $\int_{\mathbb{R}}\pi_n(t)\,\mathrm{d}\lambda(t)=0$ for $n\ge 1$, there must exist at least one point in the interior of $[a,b]$ at which π_n changes sign. Let $t_1,t_2,\dots,t_k$, $k\le n$, be all such points. If we had $k<n$, then by orthogonality

$$\int_{\mathbb{R}}\pi_n(t)\prod_{\kappa=1}^{k}(t-t_\kappa)\,\mathrm{d}\lambda(t)=0.$$

This, however, is impossible since the integrand has constant sign. Therefore, $k=n$. □

Theorem 1.20 *The zeros of* π_{n+1} *alternate with those of* π_n, *that is,*

$$\tau_{n+1}^{(n+1)}<\tau_n^{(n)}<\tau_n^{(n+1)}<\tau_{n-1}^{(n)}<\cdots<\tau_1^{(n)}<\tau_1^{(n+1)}, \tag{1.2.3}$$

where $\tau_i^{(n+1)}$, $\tau_k^{(n)}$ *are the zeros in descending order of* π_{n+1} *and* π_n, *respectively.*

Proof See the Remark in §1.3.3. □

Theorem 1.21 *In any open interval* (c,d) *in which* $\mathrm{d}\lambda\equiv 0$ *there can be at most one zero of* $\pi_n(\,\cdot\,;\mathrm{d}\lambda)$.

Proof By contradiction. Suppose there are two zeros $\tau_i^{(n)}\ne\tau_j^{(n)}$ in (c,d), and let all the others, within (c,d) or without, be $\tau_k^{(n)}$. Then,

$$\int_{\mathbb{R}}\pi_n(t;\mathrm{d}\lambda)\prod_{k\ne i,j}(t-\tau_k^{(n)})\,\mathrm{d}\lambda(t)=\int_{\mathbb{R}}\prod_{k\ne i,j}(t-\tau_k^{(n)})^2\cdot(t-\tau_i^{(n)})(t-\tau_j^{(n)})\,\mathrm{d}\lambda(t)>0,$$

since the integrand is nonnegative outside of (c,d). This contradicts orthogonality of π_n to polynomials of lower degree. □

1.2.3 *Discrete orthogonality*

The zeros of π_n, as will be seen in §1.4 (see the paragraph preceding §1.4.2), are the nodes τ_ν^G of the n-point Gauss quadrature rule (1.4.7), which is exact for polynomials of degree $\le 2n-1$. By applying this quadrature rule to the orthogonality relation (1.1.8), one obtains the following discrete orthogonality property.

Theorem 1.22 *The first n orthogonal polynomials $\pi_k(\,\cdot\,) = \pi_k(\,\cdot\,;\mathrm{d}\lambda)$, $k = 0,1,\dots,n-1$, are discrete orthogonal in the sense*

$$\sum_{\nu=1}^{n} \lambda_\nu^G \pi_k(\tau_\nu^G)\pi_\ell(\tau_\nu^G) = \delta_{k\ell}\|\pi_k\|_{\mathrm{d}\lambda}^2, \quad k,\ell = 0,1,\dots,n-1, \tag{1.2.4}$$

where $\delta_{k\ell}$ is the Kronecker delta and τ_ν^G, λ_ν^G are the nodes and weights of the n-point Gauss quadrature formula (1.4.7).

From the Gauss–Lobatto quadrature rule (1.4.22) and its error term (1.4.24), one similarly obtains

Theorem 1.23 *If $\mathrm{d}\lambda$ is supported on the finite interval $[a,b]$, then the first $n+2$ (monic) orthogonal polynomials $\pi_k(\,\cdot\,) = \pi_k(\,\cdot\,;\mathrm{d}\lambda)$, $k = 0,1,\dots,n+1$, are discrete orthogonal in the sense*

$$\begin{aligned}\lambda_0^L \pi_k(a)\pi_\ell(a) + \sum_{\nu=1}^{n} \lambda_\nu^L \pi_k(\tau_\nu^L)\pi_\ell(\tau_\nu^L) + \lambda_{n+1}^L \pi_k(b)\pi_\ell(b) \\ = \delta_{kl}\|\pi_k\|_{\mathrm{d}\lambda}^2 + \delta_{k,n+1}\delta_{\ell,n+1}\gamma_n,\end{aligned} \tag{1.2.5}$$

where τ_ν^L, λ_ν^L are the nodes and weights of the $(n+2)$-point Gauss–Lobatto quadrature formula (1.4.22) and

$$\gamma_n = \int_a^b [\pi_n(t;\mathrm{d}\lambda_{a,b})]^2\,\mathrm{d}\lambda_{a,b}(t), \quad \mathrm{d}\lambda_{a,b}(t) = (t-a)(b-t)\,\mathrm{d}\lambda(t). \tag{1.2.6}$$

The extra term on the right of (1.2.5) comes from the fact that the remainder $R_n^{a,b}(f)$ in (1.4.22) is not zero when f is a monic polynomial of degree $2n+2$, but equal to $-\gamma_n$.

1.2.4 *Extremal properties*

The set of monic polynomials of degree n will be denoted by $\mathbb{P}_n^\circ$.

Theorem 1.24 *For any monic polynomial $\pi \in \mathbb{P}_n^\circ$ there holds*

$$\int_{\mathbb{R}} \pi^2(t)\,\mathrm{d}\lambda(t) \ge \int_{\mathbb{R}} \pi_n^2(t;\mathrm{d}\lambda)\,\mathrm{d}\lambda(t), \tag{1.2.7}$$

with equality if and only if $\pi = \pi_n$. In other words, π_n minimizes the integral on the left over all $\pi \in \mathbb{P}_n^\circ$:

$$\min_{\pi\in\mathbb{P}_n^\circ} \int_{\mathbb{R}} \pi^2(t)\,\mathrm{d}\lambda(t) = \int_{\mathbb{R}} \pi_n^2(t;\mathrm{d}\lambda)\,\mathrm{d}\lambda(t). \tag{1.2.8}$$

Proof By Lemma 1.5, the polynomial π can be represented in terms of the orthogonal polynomials $\pi_0, \pi_1 \ldots, \pi_n$ as

$$\pi(t) = \pi_n(t) + \sum_{k=0}^{n-1} c_k \pi_k(t). \tag{1.2.9}$$

Therefore,

$$\int_{\mathbb{R}} \pi^2(t)\, \mathrm{d}\lambda(t) = \int_{\mathbb{R}} \pi_n^2(t)\, \mathrm{d}\lambda(t) + \sum_{k=0}^{n-1} c_k^2 \int_{\mathbb{R}} \pi_k^2(t)\, \mathrm{d}\lambda(t).$$

This establishes inequality (1.2.7) and equality if and only if $c_0 = c_1 = \cdots = c_{n-1} = 0$, that is, $\pi = \pi_n$. □

Another way of viewing the result of Theorem 1.24 is to consider the left-hand integral in (1.2.8) a function $\phi(a_0, a_1, \ldots, a_{n-1})$ of the coefficients in $\pi(t) = t^n + \sum_{k=0}^{n-1} a_k t^k$. Setting the partial derivative with respect to each a_k equal to zero yields

$$\int_{\mathbb{R}} \pi(t) t^k\, \mathrm{d}\lambda(t) = 0, \quad k = 0, 1, \ldots, n-1, \tag{1.2.10}$$

which are precisely the conditions of orthogonality that $\pi = \pi_n$ must satisfy. Moreover, the Hessian matrix of ϕ is twice the Hankel matrix $\boldsymbol{M}_n$ in (1.1.5), which by Theorem 1.2 is positive definite, confirming the minimality of π_n.

The extremal property (1.2.8) can be generalized to arbitrary powers $p > 1$.

Theorem 1.25 *Let $1 < p < \infty$. Then, the extremal problem of determining*

$$\min_{\pi \in \mathbb{P}_n^\circ} \int_{\mathbb{R}} |\pi(t)|^p\, \mathrm{d}\lambda(t) \tag{1.2.11}$$

has a unique solution $\pi_n^*(\,\cdot\,; \mathrm{d}\lambda)$.

Proof Seeking the minimum in (1.2.11) is equivalent to the problem of approximating t^n best by polynomials of degree $\le n-1$ in the p-norm $\|u\|_p = \left(\int_{\mathbb{R}} |u|^p\, d\lambda\right)^{1/p}$. It is known from approximation theory (cf., e.g. Davis (1975, Chapter VII)) that this has a unique solution. □

An interesting special case of Theorem 1.25 is $p = 2s + 2$, where $s \ge 0$ is an integer. The extremal polynomial of Theorem 1.25 is then denoted by

$$\pi_n^*(\,\cdot\,; \mathrm{d}\lambda) = \pi_{n,s}(\,\cdot\,; \mathrm{d}\lambda). \tag{1.2.12}$$

In analogy to (1.2.8) and (1.2.10), one finds that $\pi_{n,s}$ must satisfy

$$\int_{\mathbb{R}} \pi_{n,s}^{2s+1}(t) t^k\, \mathrm{d}\lambda(t) = 0, \quad k = 0, 1, \ldots, n-1. \tag{1.2.13}$$

Thus, the $(2s+1)$st power of $\pi_{n,s}$ must be orthogonal to all polynomials of lower degree. This is referred to as *power orthogonality*; the polynomials $\pi_{n,s}$ themselves are called *s-orthogonal polynomials*. Evidently, $\pi_{n,0} = \pi_n$.

Theorem 1.26 *All zeros of* $\pi_{n,s}(\,\cdot\,) = \pi_{n,s}(\,\cdot\,;\mathrm{d}\lambda)$ *are real, simple, and contained in the interior of the support interval of* $\mathrm{d}\lambda$. *The zeros of* $\pi_{n+1,s}$ *alternate with those of* $\pi_{n,s}$.

Proof The proof of the first part is analogous to the proof of Theorem 1.19. For the second part, see Milovanović (2001, Theorem 2.2). □

1.3 Three-term recurrence relation

The three-term recurrence relation satisfied by orthogonal polynomials is arguably the single most important piece of information for the constructive and computational use of orthogonal polynomials. Apart from its obvious use in generating values of orthogonal polynomials and their derivatives, both within and without the spectrum of the measure, knowledge of the recursion coefficients (i) allows the zeros of orthogonal polynomials to be readily computed as eigenvalues of a symmetric tridiagonal matrix, and with them the all-important Gaussian quadrature rule, (ii) yields immediately the normalization coefficients needed to pass from monic orthogonal to orthonormal polynomials, (iii) opens access to polynomials of the second kind and related continued fractions, and (iv) allows an efficient evaluation of expansions in orthogonal polynomials. Much of this book, therefore, is devoted to computing the coefficients of the three-term recurrence relation in cases where they are not known explicitly.

The principal reason why there exists a three-term recurrence relation is the shift property

$$(tu, v)_{\mathrm{d}\lambda} = (u, tv)_{\mathrm{d}\lambda} \quad \text{for all } u, v \in \mathbb{P} \tag{1.3.1}$$

obviously enjoyed by the inner product (1.1.2). There are other inner products, even positive definite ones, that do not satisfy (1.3.1). Among them, inner products of Sobolev type (see §1.7) and Hermitian inner products on the unit circle are the most prominent ones. In these cases, recurrence relations still exist, but they are no longer of the simple three-term variety.

1.3.1 *Monic orthogonal polynomials*

Theorem 1.27 *Let* $\pi_k(\,\cdot\,) = \pi_k(\,\cdot\,;\mathrm{d}\lambda)$, $k = 0, 1, 2, \ldots$, *be the monic orthogonal polynomials with respect to the measure* $\mathrm{d}\lambda$ (cf. Definition 1.3). *Then,*

$$\begin{gathered}\pi_{k+1}(t) = (t - \alpha_k)\pi_k(t) - \beta_k \pi_{k-1}(t), \quad k = 0, 1, 2, \ldots, \\ \pi_{-1}(t) = 0, \quad \pi_0(t) = 1,\end{gathered} \tag{1.3.2}$$

where

$$\alpha_k = \frac{(t\pi_k, \pi_k)_{\mathrm{d}\lambda}}{(\pi_k, \pi_k)_{\mathrm{d}\lambda}}, \quad k = 0, 1, 2, \ldots, \tag{1.3.3}$$

$$\beta_k = \frac{(\pi_k, \pi_k)_{\mathrm{d}\lambda}}{(\pi_{k-1}, \pi_{k-1})_{\mathrm{d}\lambda}}, \quad k = 1, 2, \ldots\ . \tag{1.3.4}$$

The index range is infinite, $k \le \infty$, *or finite,* $k \le d - 1$, *depending on whether the inner product* $(\,\cdot\,,\,\cdot\,)_{\mathrm{d}\lambda}$ *is positive definite on* $\mathbb{P}$ *resp. on* $\mathbb{P}_d$ *but not on* $\mathbb{P}_n$, $n > d$ (cf. Theorems 1.6–1.8).

Proof Since $\pi_{k+1} - t\pi_k$ is a polynomial of degree $\leq k$, by Lemma 1.5 one can write

$$\pi_{k+1}(t) - t\pi_k(t) = -\alpha_k \pi_k(t) - \beta_k \pi_{k-1}(t) + \sum_{j=0}^{k-2} \gamma_{kj} \pi_j(t) \tag{1.3.5}$$

for certain constants α_k, β_k, and γ_{kj}, where $\pi_{-1}(t) = 0$ (for $k = 0$) and empty sums (for $k = 0$ and 1) are understood to be zero. Taking the inner product of both sides with π_k yields, by orthogonality,

$$-(t\pi_k, \pi_k) = -\alpha_k(\pi_k, \pi_k),$$

that is,

$$\alpha_k = \frac{(t\pi_k, \pi_k)}{(\pi_k, \pi_k)}\,.$$

This proves (1.3.3). Relation (1.3.4) for β_k is obtained by taking the inner product with π_{k-1} ($k \geq 1$),

$$-(t\pi_k, \pi_{k-1}) = -\beta_k(\pi_{k-1}, \pi_{k-1})$$

and simplifying. Indeed, $(t\pi_k, \pi_{k-1}) = (\pi_k, t\pi_{k-1}) = (\pi_k, \pi_k + \cdots)$, where dots stand for a polynomial of degree $< k$, and thus $(t\pi_k, \pi_{k-1}) = (\pi_k, \pi_k)$, giving

$$\beta_k = \frac{(\pi_k, \pi_k)}{(\pi_{k-1}, \pi_{k-1})}\,.$$

Finally, taking the inner product of both sides of (1.3.5) with π_i, $i < k-1$, yields

$$-(t\pi_k, \pi_i) = \gamma_{ki}(\pi_i, \pi_i).$$

It is at this point where the basic property (1.3.1) plays out its crucial role: one has $(t\pi_k, \pi_i) = (\pi_k, t\pi_i)$, which vanishes by orthogonality, since $t\pi_i \in \mathbb{P}_{k-1}$. Thus, $\gamma_{ki} = 0$ for $i < k - 1$. This establishes (1.3.2). □

Remark to Theorem 1.27 If the index range in Theorem 1.27 is finite, $k \leq d-1$, then (1.3.3) and (1.3.4) are still meaningful for $k = d$, and $\beta_d > 0$, but the polynomial π_{d+1} defined by (1.3.2) for $k = d$ has norm 0, $\|\pi_{d+1}\| = 0$; see the proof of Theorem 1.7.

The coefficients in the three-term recurrence relation (1.3.2) will be denoted by $\alpha_k = \alpha_k(\mathrm{d}\lambda)$ and $\beta_k = \beta_k(\mathrm{d}\lambda)$ if the measure $\mathrm{d}\lambda$ is to be evidenced explicitly. Although β_0 in (1.3.2) can be arbitrary, since it multiplies $\pi_{-1} = 0$, it is convenient for later purposes to define

$$\beta_0(\mathrm{d}\lambda) = (\pi_0, \pi_0) = \int_{\mathbb{R}} \mathrm{d}\lambda(t). \tag{1.3.6}$$

Note from (1.3.4) and (1.3.6) that all β_k are positive and

$$\|\pi_n\|^2 = \beta_n \beta_{n-1} \cdots \beta_1 \beta_0, \quad n = 0, 1, 2, \ldots\,. \tag{1.3.7}$$

There is a converse of Theorem 1.27, usually attributed to Favard (but anticipated by a number of mathematicians as far back as Stieltjes; cf. Marcellán and

Álvarez–Nodarse (2001)), which says that any (infinite) sequence of polynomials $\pi_0, \pi_1, \pi_2, \ldots$ satisfying a three-term recurrence relation (1.3.2) with all β_k positive is orthogonal with respect to some positive measure with infinite support (cf., e.g. Natanson (1965, Chapter VIII, §6)).

Theorem 1.28 *Let the support interval* $[a, b]$ *of* $\mathrm{d}\lambda$ *be finite. Then,*

$$a < \alpha_k(\mathrm{d}\lambda) < b, \quad k = 0, 1, 2, \ldots, \tag{1.3.8}$$

$$0 < \beta_k(\mathrm{d}\lambda) \leq \max(a^2, b^2), \quad k = 1, 2, \ldots, \tag{1.3.9}$$

where the index range is $k \leq \infty$ *resp.* $k \leq d$*, with* d *as in Theorem 1.27.*

Proof The first relation, (1.3.8), follows immediately from (1.3.3) by noting that $a \leq t \leq b$ for t in the support of $\mathrm{d}\lambda$. It remains to prove the upper bound in (1.3.9).

From

$$\|\pi_k\|^2 = (\pi_k, \pi_k) = |(t\pi_{k-1}, \pi_k)|$$

and Schwarz's inequality (1.1.4), one gets

$$\|\pi_k\|^2 \leq \max(|a|, |b|)\|\pi_{k-1}\| \cdot \|\pi_k\|.$$

Dividing both sides by $\|\pi_k\|$ and squaring yields the assertion, since $\beta_k = \|\pi_k\|^2/\|\pi_{k-1}\|^2$ by (1.3.4). □

The *Szegö class* $\mathcal{S}$ of (absolutely continuous) measures supported on $[-1, 1]$ consists of measures $\mathrm{d}\lambda(t) = w(t)\,\mathrm{d}t$ such that

$$\int_{-1}^{1} \frac{\ln w(t)}{\sqrt{1-t^2}}\,\mathrm{d}t > -\infty. \tag{1.3.10}$$

For such measures it is known that

$$\lim_{k\to\infty} \alpha_k(\mathrm{d}\lambda) = 0, \quad \lim_{k\to\infty} \beta_k(\mathrm{d}\lambda) = \tfrac{1}{4} \qquad (\mathrm{d}\lambda \in \mathcal{S}); \tag{1.3.11}$$

cf. Szegö (1975, eqns (12.7.4) and (12.7.6)).

1.3.2 *Orthonormal polynomials*

With $\tilde{\pi}_k(\,\cdot\,) = \tilde{\pi}_k(\,\cdot\,; \mathrm{d}\lambda)$ denoting the orthonormal polynomials (cf. Definition 1.3), one has

$$\pi_k(t) = \|\pi_k\|\,\tilde{\pi}_k(t), \quad k = 0, 1, 2, \ldots\ . \tag{1.3.12}$$

Theorem 1.29 *Let* $\tilde{\pi}_k(\,\cdot\,) = \tilde{\pi}_k(\,\cdot\,; \mathrm{d}\lambda)$*,* $k = 0, 1, 2, \ldots$*, be the orthonormal polynomials with respect to the measure* $\mathrm{d}\lambda$*. Then,*

$$\begin{aligned} \sqrt{\beta_{k+1}}\tilde{\pi}_{k+1}(t) &= (t - \alpha_k)\tilde{\pi}_k(t) - \sqrt{\beta_k}\tilde{\pi}_{k-1}(t), \quad k = 0, 1, 2, \ldots, \\ \tilde{\pi}_{-1}(t) &= 0, \quad \tilde{\pi}_0(t) = 1/\sqrt{\beta_0}, \end{aligned} \tag{1.3.13}$$

where the α*s and* β*s are given by (1.3.3), (1.3.4), and (1.3.6). The index range is the same as in Theorem 1.27.*

Proof Inserting (1.3.12) into (1.3.2), dividing by $\|\pi_{k+1}\|$, and noting (1.3.4) yields

$$\tilde{\pi}_{k+1}(t) = (t-\alpha_k)\frac{\tilde{\pi}_k(t)}{\sqrt{\beta_{k+1}}} - \beta_k \frac{\tilde{\pi}_{k-1}(t)}{\sqrt{\beta_{k+1}\beta_k}}\,.$$

Multiplying through by $\sqrt{\beta_{k+1}}$ gives the three-term recurrence relation in (1.3.13). The starting values follow from those in (1.3.2), noting from (1.3.12) and (1.3.7) with $k=0$ that $1 = \sqrt{\beta_0}\tilde{\pi}_0$. □

Definition 1.30 *If the index range in Theorems 1.27 and 1.29 is infinite, the* Jacobi matrix *associated with the measure* $\mathrm{d}\lambda$ *is the infinite, symmetric, tridiagonal matrix*

$$\boldsymbol{J}_\infty = \boldsymbol{J}_\infty(\mathrm{d}\lambda) := \begin{bmatrix} \alpha_0 & \sqrt{\beta_1} & & & 0 \\ \sqrt{\beta_1} & \alpha_1 & \sqrt{\beta_2} & & \\ & \sqrt{\beta_2} & \alpha_2 & \sqrt{\beta_3} & \\ & & \ddots & \ddots & \ddots \\ 0 & & & & \end{bmatrix}. \tag{1.3.14}$$

Its $n \times n$ leading principal minor matrix is denoted by

$$\boldsymbol{J}_n = \boldsymbol{J}_n(\mathrm{d}\lambda) := [\boldsymbol{J}_\infty(\mathrm{d}\lambda)]_{[1:n,1:n]}. \tag{1.3.15}$$

If the index range in Theorem 1.29 is finite, $k \le d-1$, then $\boldsymbol{J}_n$ is well defined for $0 \le n \le d$.

If the first n equations of (1.3.13) are written in the form

$$t\tilde{\pi}_k(t) = \sqrt{\beta_k}\tilde{\pi}_{k-1}(t) + \alpha_k\tilde{\pi}_k(t) + \sqrt{\beta_{k+1}}\tilde{\pi}_{k+1}(t), \quad k = 0, 1, \ldots, n-1, \tag{1.3.16}$$

and one lets

$$\tilde{\boldsymbol{\pi}}(t) = [\tilde{\pi}_0(t), \tilde{\pi}_1(t), \ldots, \tilde{\pi}_{n-1}(t)]^{\mathrm{T}}, \tag{1.3.17}$$

then (1.3.16) may be expressed in matrix form as

$$t\tilde{\boldsymbol{\pi}}(t) = \boldsymbol{J}_n(\mathrm{d}\lambda)\tilde{\boldsymbol{\pi}}(t) + \sqrt{\beta_n}\tilde{\pi}_n(t)\boldsymbol{e}_n, \tag{1.3.18}$$

where $\boldsymbol{e}_n = [0, 0, \ldots, 1]^{\mathrm{T}}$ is the nth coordinate vector in $\mathbb{R}^n$.

Theorem 1.31 *The zeros $\tau_\nu^{(n)}$ of $\pi_n(\,\cdot\,;\mathrm{d}\lambda)$ (or $\tilde{\pi}_n(\,\cdot\,;\mathrm{d}\lambda)$) are the eigenvalues of the Jacobi matrix $\boldsymbol{J}_n(\mathrm{d}\lambda)$ of order n, and $\tilde{\boldsymbol{\pi}}(\tau_\nu^{(n)})$ are corresponding eigenvectors.*

Proof Both assertions follow immediately from (1.3.18) by putting $t = \tau_\nu^{(n)}$ and noting that $\tilde{\boldsymbol{\pi}}(\tau_\nu^{(n)}) \neq \boldsymbol{0}$, the first component of $\tilde{\boldsymbol{\pi}}(\tau_\nu^{(n)})$ being $1/\sqrt{\beta_0}$. □

Corollary to Theorem 1.31 Let $\boldsymbol{v}_\nu$ denote the normalized eigenvector of $\boldsymbol{J}_n(\mathrm{d}\lambda)$ corresponding to the eigenvalue $\tau_\nu^{(n)}$,

$$\boldsymbol{J}_n(\mathrm{d}\lambda)\boldsymbol{v}_\nu = \tau_\nu^{(n)}\boldsymbol{v}_\nu, \quad \boldsymbol{v}_\nu^{\mathrm{T}}\boldsymbol{v}_\nu = 1, \tag{1.3.19}$$

and let $\boldsymbol{v}_{\nu,1}$ denote its first component. Then,

$$\beta_0 \boldsymbol{v}_{\nu,1}^2 = \frac{1}{\sum_{k=0}^{n-1} [\tilde{\pi}_k(\tau_\nu^{(n)})]^2}, \quad \nu = 1, 2, \ldots, n. \tag{1.3.20}$$

Proof Claim (1.3.20) follows from

$$\boldsymbol{v}_\nu = \left(\sum_{k=0}^{n-1} [\tilde{\pi}_k(\tau_\nu^{(n)})]^2 \right)^{-1/2} \tilde{\boldsymbol{\pi}}(\tau_\nu^{(n)}), \quad \nu = 1, 2, \ldots, n,$$

by comparing the first component on each side and squaring, noting from (1.3.13) that $\tilde{\pi}_0 = 1/\sqrt{\beta_0}$. □

1.3.3 *Christoffel–Darboux formulae*

A simple, but important, consequence of the three-term recurrence relation (1.3.13) is the following theorem.

Theorem 1.32 (Christoffel–Darboux formula) *Let* $\tilde{\pi}_k(\,\cdot\,) = \tilde{\pi}_k(\,\cdot\,;\mathrm{d}\lambda)$ *denote the orthonormal polynomials with respect to the measure* $\mathrm{d}\lambda$*. Then,*

$$\sum_{k=0}^{n} \tilde{\pi}_k(x)\tilde{\pi}_k(t) = \sqrt{\beta_{n+1}}\, \frac{\tilde{\pi}_{n+1}(x)\tilde{\pi}_n(t) - \tilde{\pi}_n(x)\tilde{\pi}_{n+1}(t)}{x - t} \tag{1.3.21}$$

and

$$\sum_{k=0}^{n} [\tilde{\pi}_k(t)]^2 = \sqrt{\beta_{n+1}}\, [\tilde{\pi}'_{n+1}(t)\tilde{\pi}_n(t) - \tilde{\pi}'_n(t)\tilde{\pi}_{n+1}(t)]. \tag{1.3.22}$$

Proof Multiplying the recurrence relation (1.3.13) by $\tilde{\pi}_k(x)$ and subtracting the resulting relation from the one with x and t interchanged yields

$$\begin{aligned}(x - t)\tilde{\pi}_k(x)\tilde{\pi}_k(t) = {} & \sqrt{\beta_{k+1}}\, [\tilde{\pi}_{k+1}(x)\tilde{\pi}_k(t) - \tilde{\pi}_k(x)\tilde{\pi}_{k+1}(t)] \\ & - \sqrt{\beta_k}\, [\tilde{\pi}_k(x)\tilde{\pi}_{k-1}(t) - \tilde{\pi}_{k-1}(x)\tilde{\pi}_k(t)].\end{aligned}$$

Summing both sides from $k = 0$ to $k = n$ and observing $\tilde{\pi}_{-1} = 0$ and the telescoping nature of the summation on the right gives (1.3.21). Taking the limit $x \to t$ gives (1.3.22). □

Corollary to Theorem 1.32 Let $\pi_k(\,\cdot\,) = \pi_k(\,\cdot\,;\mathrm{d}\lambda)$ denote the monic orthogonal polynomials with respect to the measure $\mathrm{d}\lambda$. Then,

$$\sum_{k=0}^{n} \beta_n\beta_{n-1}\cdots\beta_{k+1}\pi_k(x)\pi_k(t) = \frac{\pi_{n+1}(x)\pi_n(t) - \pi_n(x)\pi_{n+1}(t)}{x - t}. \tag{1.3.23}$$

Proof Put $\tilde{\pi}_k = \pi_k/\|\pi_k\|$ in (1.3.21) and use $\sqrt{\beta_{n+1}} = \|\pi_{n+1}\|/\|\pi_n\|$ along with (1.3.7). □

Remark From (1.3.22) one obtains the useful inequality

$$\tilde{\pi}'_{n+1}(t)\tilde{\pi}_n(t) - \tilde{\pi}'_n(t)\tilde{\pi}_{n+1}(t) > 0. \tag{1.3.24}$$

It provides, for example, a quick proof of Theorem 1.20. Indeed, let τ and σ be consecutive zeros of $\tilde{\pi}_n$, so that $\tilde{\pi}'_n(\tau)\tilde{\pi}'_n(\sigma) < 0$. Then, $-\tilde{\pi}'_n(\tau)\tilde{\pi}_{n+1}(\tau) > 0$ and $-\tilde{\pi}'_n(\sigma)\tilde{\pi}_{n+1}(\sigma) > 0$ by (1.3.24), implying that $\tilde{\pi}_{n+1}$ at τ and σ has opposite signs. Therefore, there is at least one zero of $\tilde{\pi}_{n+1}$ between τ and σ. This accounts for at least $n-1$ zeros of $\tilde{\pi}_{n+1}$. There are, however, two additional zeros of $\tilde{\pi}_{n+1}$, one to the right of the largest zero $\tau_1^{(n)}$ of $\tilde{\pi}_n$ and one to the left of the smallest, $\tau_n^{(n)}$. This is so because $\tilde{\pi}'_n(\tau_1^{(n)}) > 0$ and, again by (1.3.24), $\tilde{\pi}_{n+1}(\tau_1^{(n)}) < 0$. Thus, $\tilde{\pi}_{n+1}$ must vanish to the right of $\tau_1^{(n)}$ since $\tilde{\pi}_{n+1}(t) > 0$ for t sufficiently large. A similar argument holds at $\tau_n^{(n)}$. This proves (1.2.3).

1.3.4 *Continued fractions*

Historically, orthogonal polynomials—in substance if not in name—arose as denominators of a certain continued fraction. It seems appropriate, therefore, to briefly pursue this connection with continued fractions. Not only the denominators, but also the numerators of the continued fraction are of interest, as they give rise to a series of related orthogonal polynomials.

Assume $\mathrm{d}\lambda$ to be a positive measure with infinitely many points of increase, and let $\alpha_k = \alpha_k(\mathrm{d}\lambda)$, $\beta_k = \beta_k(\mathrm{d}\lambda)$, $k = 0, 1, 2, \ldots$, denote the coefficients in the three-term recurrence relation for the orthogonal polynomials $\pi_k(\,\cdot\,) = \pi_k(\,\cdot\,;\mathrm{d}\lambda)$, with β_0 as defined in (1.3.6).

Definition 1.33 *The* Jacobi continued fraction *associated with the measure* $\mathrm{d}\lambda$ *is*

$$\mathcal{J} = \mathcal{J}(t;\mathrm{d}\lambda) = \frac{\beta_0}{t-\alpha_0-}\,\frac{\beta_1}{t-\alpha_1-}\,\frac{\beta_2}{t-\alpha_2-}\,\cdots\,. \tag{1.3.25}$$

Its nth *convergent is denoted by*

$$\frac{A_n}{B_n} = \frac{A_n(t;\mathrm{d}\lambda)}{B_n(t;\mathrm{d}\lambda)} = \frac{\beta_0}{t-\alpha_0-}\,\frac{\beta_1}{t-\alpha_1-}\,\cdots\,\frac{\beta_{n-1}}{t-\alpha_{n-1}}, \quad n = 1, 2, 3, \ldots\,. \tag{1.3.26}$$

From the theory of continued fractions (see, e.g. Jones and Thron (1980, §2.1)), it is well known that the numerators A_n and denominators B_n satisfy the recurrence relations

$$\begin{gathered} A_{k+1} = (t-\alpha_k)A_k - \beta_k A_{k-1}, \quad k = 1, 2, \ldots, \\ A_0 = 0, \quad A_1 = \beta_0 \end{gathered} \tag{1.3.27}$$

resp.

$$\begin{gathered} B_{k+1} = (t - \alpha_k)B_k - \beta_k B_{k-1}, \quad k = 0, 1, 2, \ldots, \\ B_{-1} = 0, \quad B_0 = 1. \end{gathered} \tag{1.3.28}$$

Since (1.3.28) is identical with the recurrence relation for the monic orthogonal polynomials, the following theorem is self-evident.

Theorem 1.34 *The denominators B_k of the Jacobi continued fraction (1.3.25) are precisely the monic orthogonal polynomials π_k,*

$$B_k(t; \mathrm{d}\lambda) = \pi_k(t; \mathrm{d}\lambda), \quad k = 0, 1, 2, \ldots \ . \tag{1.3.29}$$

As regards the numerators A_n, a simple inductive argument based on (1.3.27) reveals that $\beta_0^{-1} A_{k+1}(\,\cdot\,; \mathrm{d}\lambda)$ is a monic polynomial of degree k which does not depend on β_0.

Definition 1.35 *The polynomial*

$$\pi_k^{[1]}(t; \mathrm{d}\lambda) = \beta_0^{-1} A_{k+1}(t; \mathrm{d}\lambda) \tag{1.3.30}$$

is called the (first) numerator polynomial *of degree k associated with the measure* $\mathrm{d}\lambda$.

Theorem 1.36 *The numerator polynomials $\pi_k^{[1]}(\,\cdot\,) = \pi_k^{[1]}(\,\cdot\,; \mathrm{d}\lambda)$ satisfy the three-term recurrence relation*

$$\begin{gathered} \pi_{k+1}^{[1]}(t) = (t - \alpha_{k+1})\pi_k^{[1]}(t) - \beta_{k+1}\pi_{k-1}^{[1]}(t), \quad k = 0, 1, 2, \ldots, \\ \pi_{-1}^{[1]}(t) = 0, \quad \pi_0^{[1]}(t) = 1, \end{gathered} \tag{1.3.31}$$

where $\alpha_{k+1} = \alpha_{k+1}(\mathrm{d}\lambda)$, $\beta_{k+1} = \beta_{k+1}(\mathrm{d}\lambda)$.

Proof This is an immediate consequence of (1.3.27) and (1.3.30). □

Since $\alpha_{k+1} \in \mathbb{R}$ and $\beta_{k+1} > 0$ for $k = 0, 1, 2, \ldots$, it follows from (1.3.31) and Favard's theorem that the numerator polynomials are also orthogonal with respect to a positive measure $\mathrm{d}\lambda^{[1]}$. In general, however, $\mathrm{d}\lambda^{[1]}$ is not known.

Example 1.37 (Chihara, 1978, Chapter VI, eqn (12.4)) For the Legendre measure $\mathrm{d}\lambda(t) = \mathrm{d}t$ on $[-1, 1]$ (cf. §1.5.1), one has

$$\mathrm{d}\lambda^{[1]}(t) = \frac{\mathrm{d}t}{\left[\ln \dfrac{1+t}{1-t}\right]^2 + \pi^2}, \quad -1 < t < 1.$$

Theorem 1.36 suggests to define numerator polynomials of higher order.

Definition 1.38 *The* numerator polynomials $\pi_k^{[s]}(\,\cdot\,) = \pi_k^{[s]}(\,\cdot\,; \mathrm{d}\lambda)$ of order $s \geq 0$ *are defined to be the solution of the three-term recurrence relation*

$$\begin{gathered} \pi_{k+1}^{[s]}(t) = (t - \alpha_{k+s})\pi_k^{[s]}(t) - \beta_{k+s}\pi_{k-1}^{[s]}(t), \quad k = 0, 1, 2, \ldots, \\ \pi_{-1}^{[s]}(t) = 0, \quad \pi_0^{[s]}(t) = 1, \end{gathered} \tag{1.3.32}$$

where $\alpha_{k+s} = \alpha_{k+s}(\mathrm{d}\lambda)$, $\beta_{k+s} = \beta_{k+s}(\mathrm{d}\lambda)$. Evidently, $\pi_k^{[0]} = \pi_k$.

Although the measure of orthogonality $\mathrm{d}\lambda^{[s]}$ of the numerator polynomials $\pi_k^{[s]}$ is not known, its Cauchy integral (cf. §2.3) can be expressed in terms of Cauchy integrals of $\mathrm{d}\lambda$ (Van Assche, 1991, eqn (3.7))

$$\int_{\mathbb{R}} \frac{\mathrm{d}\lambda^{[s]}(t)}{z-t} = \frac{1}{\beta_s}\,\frac{\rho_s(z)}{\rho_{s-1}(z)}, \quad \rho_k(z) = \int_{\mathbb{R}} \frac{\pi_k(t;\mathrm{d}\lambda)\,\mathrm{d}\lambda(t)}{z-t}\,,$$

which, in fact, may be used to recover $\mathrm{d}\lambda^{[s]}$ by the Stieltjes–Perron inversion formula (cf. Example 2.50).

Also, the Stieltjes polynomial $\pi_{n+1}^K(\,\cdot\,;\mathrm{d}\lambda)$ in the theory of Gauss–Kronrod quadrature (cf. §3.1.2) can be expressed in terms of $\mathrm{d}\lambda^{[n+1]}$ (Peherstorfer and Petras, 2000, Theorem 3).

1.3.5 *The recurrence relation outside the support interval*

It is of interest to consider the Jacobi continued fraction (1.3.25) for complex $z \in \mathbb{C}\backslash[a,b]$ outside the support interval $[a,b]$ of $\mathrm{d}\lambda$. According to Theorem 1.34, (1.3.26), and Definition 1.35, replacing t by z, one has

$$\frac{\beta_0}{z-\alpha_0-}\,\frac{\beta_1}{z-\alpha_1-}\cdots\frac{\beta_{n-1}}{z-\alpha_{n-1}} = \frac{\sigma_n(z;\mathrm{d}\lambda)}{\pi_n(z;\mathrm{d}\lambda)}\,, \quad n=1,2,3,\ldots, \tag{1.3.33}$$

where $\pi_n(\,\cdot\,;\mathrm{d}\lambda)$ is the monic orthogonal polynomial of degree n, and

$$\sigma_n(z;\mathrm{d}\lambda) = \beta_0\pi_{n-1}^{[1]}(z;\mathrm{d}\lambda), \tag{1.3.34}$$

with $\pi_{n-1}^{[1]}$ the first numerator polynomial of degree $n-1$. By Theorem 1.36, the polynomials $\sigma_k(\,\cdot\,) = \sigma_k(\,\cdot\,;\mathrm{d}\lambda)$ satisfy

$$\begin{aligned} \sigma_{k+1}(z) &= (z-\alpha_k)\sigma_k(z) - \beta_k\sigma_{k-1}(z), \quad k=1,2,3,\ldots, \\ \sigma_0(z) &= 0, \quad \sigma_1(z) = \beta_0. \end{aligned} \tag{1.3.35}$$

Recall that $\beta_0 = \int_{\mathbb{R}} \mathrm{d}\lambda(t)$. If one defines $\sigma_{-1}(z) = -1$, then (1.3.35) holds also for $k=0$.

Theorem 1.39 *The numerators in (1.3.33) are given by*

$$\sigma_n(z) = \int_{\mathbb{R}} \frac{\pi_n(z)-\pi_n(t)}{z-t}\,\mathrm{d}\lambda(t), \quad n=1,2,3,\ldots\,. \tag{1.3.36}$$

Proof It suffices to show that the integral on the right satisfies (1.3.35). As regards the starting values, this is trivial, since $\pi_0 = 1$ and $\pi_1(z) = z-\alpha_1$. To establish the rest, we use the recurrence relation of the π_ks to write

$$\begin{aligned} &\pi_{k+1}(z) - \pi_{k+1}(t) \\ &\quad = z\pi_k(z) - t\pi_k(t) - \alpha_k[\pi_k(z)-\pi_k(t)] - \beta_k[\pi_{k-1}(z)-\pi_{k-1}(t)] \\ &\quad = (z-t)\pi_k(t) + (z-\alpha_k)[\pi_k(z)-\pi_k(t)] - \beta_k[\pi_{k-1}(z)-\pi_{k-1}(t)]. \end{aligned}$$

Dividing both sides by $z-t$ and integrating yields

$$\sigma_{k+1}(z) = \int_{\mathbb{R}} \pi_k(t)\,\mathrm{d}\lambda(t) + (z-\alpha_k)\sigma_k(z) - \beta_k\sigma_{k-1}(z).$$

Since $k \geq 1$, the integral on the right vanishes by orthogonality. □

The polynomials σ_n are called the *polynomials of the second kind*, or the *associated polynomials*, with respect to the measure $\mathrm{d}\lambda$.

Let

$$F(z) = F(z;\mathrm{d}\lambda) := \int_{\mathbb{R}} \frac{\mathrm{d}\lambda(t)}{z-t}, \quad z \in \mathbb{C}\backslash[a,b]. \tag{1.3.37}$$

This is a function vanishing at infinity and analytic in the whole complex plane with the interval $[a,b]$ removed. (If $-a = b = +\infty$, then F is analytic separately in $\operatorname{Im} z > 0$ and $\operatorname{Im} z < 0$, the two branches being different in general.) To elucidate the connection between F in (1.3.37) and the continued fractions in (1.3.33), we begin by formally expanding F in descending powers of z,

$$F(z) \sim \frac{\mu_0}{z} + \frac{\mu_1}{z^2} + \frac{\mu_2}{z^3} + \cdots, \tag{1.3.38}$$

where μ_r are the moments (1.1.1) of $\mathrm{d}\lambda$. Define

$$\rho_n(z) = \rho_n(z;\mathrm{d}\lambda) := \int_{\mathbb{R}} \frac{\pi_n(t;\mathrm{d}\lambda)}{z-t}\,\mathrm{d}\lambda(t), \quad n = 0,1,2,\ldots. \tag{1.3.39}$$

Note from (1.3.36) and (1.3.37) that

$$\sigma_n(z) = \pi_n(z)F(z) - \rho_n(z). \tag{1.3.40}$$

Formal expansion of ρ_n yields

$$\rho_n(z) \sim \sum_{k=0}^{\infty} \frac{r_k}{z^{k+1}}, \quad r_k = \int_{\mathbb{R}} t^k \pi_n(t)\,\mathrm{d}\lambda(t). \tag{1.3.41}$$

By orthogonality, $r_k = 0$ for $k < n$, so that

$$\rho_n(z) = O(z^{-n-1}) \quad \text{as } z \to \infty. \tag{1.3.42}$$

It follows from (1.3.40) that

$$F(z) - \frac{\sigma_n(z)}{\pi_n(z)} = \frac{\rho_n(z)}{\pi_n(z)} = O(z^{-2n-1}) \quad \text{as } z \to \infty. \tag{1.3.43}$$

Thus, for each $n = 1,2,3,\ldots$, if σ_n/π_n or, equivalently, the continued fraction (1.3.33), is expanded in descending powers of z, the expansion agrees with that of F up to and including the term with z^{-2n}. In the language of continued fraction theory, this means that the Jacobi continued fraction (1.3.25) for $\mathrm{d}\lambda$ is

the *continued fraction "associated" with the formal power series in (1.3.38) for* $F(\,\cdot\,;\mathrm{d}\lambda)$.

The connection between the continued fraction (1.3.25) and F is actually much closer. To desribe it, one needs a simple notion from the theory of the moment problem. The *moment problem* consists in determining the measure $\mathrm{d}\lambda$ from the sequence of its moments $\mu_0, \mu_1, \mu_2, \ldots$ (see (1.1.1)).

Definition 1.40 *The moment problem for* $\mathrm{d}\lambda$ *is said to be* determined *if the measure* $\mathrm{d}\lambda$ *is uniquely determined by its moments. It is called* indeterminate *otherwise.*

Theorem 1.41 *If the moment problem for* $\mathrm{d}\lambda$ *is determined, then*

$$\lim_{n\to\infty} \frac{\sigma_n(z;\mathrm{d}\lambda)}{\pi_n(z;\mathrm{d}\lambda)} = F(z;\mathrm{d}\lambda), \quad z \in \mathbb{C}\backslash[a,b]. \tag{1.3.44}$$

Proof For a finite interval $[a,b]$, the moment problem is always determined, and Theorem 1.41 is due to Markov; see Szegö (1975, Theorem 3.5.4) or Perron (1957, Satz 4.2). For half-infinite and doubly infinite intervals $[a,b]$, the theorem is due, respectively, to Stieltjes (Perron, 1957, Satz 4.14 and Satz 4.10) and Hamburger (Perron, 1957, Satz 4.15 and Satz 4.11). □

Remark to Theorem 1.41 In the case of unbounded intervals $[a,b]$, there are sufficient conditions of Carleman for the moment problem to be determined. They are expressed in terms of the moments μ_r; cf. Shohat and Tamarkin (1943, Theorems 1.11 and 1.10, and p. 59).

Theorem 1.41 has an important consequence regarding the sequence of functions ρ_n, $n = 0, 1, 2, \ldots$, defined in (1.3.39).

Definition 1.42 *Consider the difference equation* (cf. (1.3.35))

$$y_{k+1} = (z - \alpha_k)y_k - \beta_k y_{k-1}, \quad k = 0, 1, 2, \ldots \tag{1.3.45}$$

(*where* $\alpha_k = \alpha_k(\mathrm{d}\lambda)$, $\beta_k = \beta_k(\mathrm{d}\lambda)$). *A solution* $\{f_n\}$ *of (1.3.45) is said to be* minimal *if*

$$\lim_{n\to\infty} \frac{f_n}{y_n} = 0 \tag{1.3.46}$$

for any solution $\{y_n\}$ *linearly independent of* $\{f_n\}$.

In general, a minimal solution may or may not exist. If it exists, it is uniquely determined up to a constant factor; cf. Gautschi (1967a).

Theorem 1.43 *Under the condition of Theorem 1.41, the sequence* $\rho_{-1}(z) = 1$, $\rho_n(z) = \rho_n(z;\mathrm{d}\lambda)$, $n = 0, 1, 2, \ldots$, *defined in (1.3.39), is a minimal solution of (1.3.45) if* $z \in \mathbb{C}\backslash[a,b]$.

Proof First, it follows from (1.3.40) that $\rho_n(z)$, $n \geq -1$, is a solution of (1.3.45) if we assume $\sigma_{-1}(z) = -1$. To prove minimality, it suffices to show that (1.3.46) holds for one particular solution $y_n = y_n^0$ of (1.3.45) which is linearly independent

of f_n. Indeed, every solution y_n of (1.3.45) linearly independent of f_n can be represented in the form

$$y_n = c_0 y_n^0 + c_1 f_n, \quad c_0 \neq 0.$$

Then,

$$\frac{f_n}{y_n} = \frac{f_n}{c_0 y_n^0 + c_1 f_n} = \frac{f_n/y_n^0}{c_0 + c_1 f_n/y_n^0} \to 0 \quad \text{as } n \to \infty.$$

In the case at hand, $f_n = \rho_n(z)$, and from (1.3.40) we have

$$\frac{\rho_n(z)}{\pi_n(z)} = F(z) - \frac{\sigma_n(z)}{\pi_n(z)}.$$

By Theorem 1.41, this tends to zero as $n \to \infty$, when $z \in \mathbb{C}\backslash[a,b]$, so that we can take $y_n^0 = \pi_n(z)$. □

Combining Theorem 1.43 with a well-known theorem of Pincherle (see, e.g. Gautschi (1967a, Theorem 1.1)), we can state the following corollary.

Corollary to Theorem 1.43 Under the condition of Theorem 1.41, the sequence $\rho_n(z)$, $n = -1, 0, 1, 2, \ldots$, defined in Theorem 1.43, is a minimal solution of (1.3.45), when $z \in \mathbb{C}\backslash[a,b]$, and there holds

$$\frac{\rho_n(z)}{\rho_{n-1}(z)} = \frac{\beta_n}{z-\alpha_n-} \frac{\beta_{n+1}}{z-\alpha_{n+1}-} \frac{\beta_{n+2}}{z-\alpha_{n+2}-} \cdots, \quad n = 0, 1, 2, \ldots, \ z \in \mathbb{C}\backslash[a,b]. \tag{1.3.47}$$

This expresses the "tails" of the Jacobi continued fraction $\mathcal{J}(z; \mathrm{d}\lambda)$ (cf. Definition 1.33) in terms of ratios of the minimal solution $\{\rho_n(z)\}$.

1.4 Quadrature rules

Let $\mathrm{d}\lambda$ be a measure with bounded or unbounded support, which may or may not be positive but is such that the assumptions made at the beginning of §1.1.1 are satisfied. An n-point *quadrature rule* for the measure $\mathrm{d}\lambda$ is a formula of the type

$$\int_{\mathbb{R}} f(t)\,\mathrm{d}\lambda(t) = \sum_{\nu=1}^{n} \lambda_\nu f(\tau_\nu) + R_n(f), \tag{1.4.1}$$

where the sum on the right provides an approximation to the integral on the left and R_n is the respective error. The τ_ν, assumed mutually distinct, are called the *nodes*, and λ_ν the *weights* of the quadrature rule.

Definition 1.44 *The quadrature rule (1.4.1) is said to have* degree of exactness *d if*

$$R_n(p) = 0 \quad \textit{for } p \in \mathbb{P}_d. \tag{1.4.2}$$

It is said to have precise degree of exactness *d if it has degree of exactness d but not $d+1$, that is, if (1.4.2) holds but $R_n(p) \neq 0$ for some $p \in \mathbb{P}_{d+1}$.*

A quadrature rule (1.4.1) with degree of exactness $d = n-1$ is called *interpolatory*.

1.4.1 *Interpolatory quadrature rules and beyond*

The quadrature rule (1.4.1) is interpolatory if and only if it is "obtained by interpolation," that is, by integrating the Lagrange interpolation formula

$$f(t) = \sum_{\nu=1}^{n} f(\tau_\nu)\ell_\nu(t) + r_{n-1}(f;t), \tag{1.4.3}$$

where

$$\ell_\nu(t) = \prod_{\substack{\mu=1 \\ \mu\neq\nu}}^{n} \frac{t-\tau_\mu}{\tau_\nu-\tau_\mu}\,. \tag{1.4.4}$$

(The dependence on n is suppressed in the notation for ℓ_ν.) Then,

$$\lambda_\nu = \int_{\mathbb{R}} \ell_\nu(t)\,\mathrm{d}\lambda(t),\ \nu = 1,2,\ldots,n; \quad R_n(f) = \int_{\mathbb{R}} r_{n-1}(f;t)\,\mathrm{d}\lambda(t). \tag{1.4.5}$$

Indeed, $r_{n-1}(p;t) \equiv 0$ if $p \in \mathbb{P}_{n-1}$; hence, $R_n(p) = 0$, so that $d = n-1$. Conversely, if $d = n-1$, then letting $f = \ell_\mu$ in (1.4.1), one gets $\int_{\mathbb{R}} \ell_\mu(t)\,\mathrm{d}\lambda(t) = \sum_{\nu=1}^{n} \lambda_\nu \ell_\mu(\tau_\nu) = \lambda_\mu$, $\mu = 1,2,\ldots,n$, since $\ell_\mu \in \mathbb{P}_{n-1}$ and $\ell_\mu(\tau_\nu) = \delta_{\mu\nu}$.

A prototype of an interpolatory quadrature rule is the *Newton–Cotes formula*, where $\mathrm{d}\lambda(t) = \mathrm{d}t$ on $[-1,1]$ and τ_ν are equally spaced on $[-1,1]$. The respective weights λ_ν are called *Cotes numbers*.

Evidently, given any n distinct nodes τ_ν, formula (1.4.1) can always be made interpolatory, that is, to have degree of exactness $d = n-1$. Theorem 1.45 tells us under what conditions one can do better. To formulate the theorem, it is convenient to introduce the *node polynomial*

$$\omega_n(t) = \prod_{\nu=1}^{n} (t-\tau_\nu). \tag{1.4.6}$$

Theorem 1.45 *Given an integer k with $0 \le k \le n$, the quadrature rule (1.4.1) has degree of exactness $d = n-1+k$ if and only if both of the following conditions are satisfied:*

(a) *Formula (1.4.1) is interpolatory.*
(b) *The node polynomial (1.4.6) satisfies*

$$\int_{\mathbb{R}} \omega_n(t)p(t)\,\mathrm{d}\lambda(t) = 0 \quad \textit{for all } p \in \mathbb{P}_{k-1}.$$

Proof The necessity of (a) is trivial, and that of (b) immediate, since $\omega_n p \in \mathbb{P}_{n-1+k}$ and, therefore,

$$\int_{\mathbb{R}} \omega_n(t)p(t)\,\mathrm{d}\lambda(t) = \sum_{\nu=1}^{n} \lambda_\nu \omega_n(\tau_\nu)p(\tau_\nu) = 0,$$

since $\omega_n(\tau_\nu) = 0$.

To prove the sufficiency of (a) and (b), one must show that under these conditions $R_n(p) = 0$ for any $p \in \mathbb{P}_{n-1+k}$. Given any such p, we divide it by ω_n to obtain

$$p = q\omega_n + r, \quad q \in \mathbb{P}_{k-1},\ r \in \mathbb{P}_{n-1}.$$

Then,

$$\int_{\mathbb{R}} p(t)\,\mathrm{d}\lambda(t) = \int_{\mathbb{R}} q(t)\omega_n(t)\,\mathrm{d}\lambda(t) + \int_{\mathbb{R}} r(t)\,\mathrm{d}\lambda(t).$$

The first integral on the right vanishes by (b), since $q \in \mathbb{P}_{k-1}$. The second, since $r \in \mathbb{P}_{n-1}$, equals

$$\sum_{\nu=1}^{n} \lambda_\nu r(\tau_\nu)$$

by virtue of (a). But

$$r(\tau_\nu) = p(\tau_\nu) - q(\tau_\nu)\omega_n(\tau_\nu) = p(\tau_\nu),$$

so that indeed

$$\int_{\mathbb{R}} p(t)\,\mathrm{d}\lambda(t) = \sum_{\nu=1}^{n} \lambda_\nu p(\tau_\nu),$$

that is, $R_n(p) = 0$. □

Note that (b) are conditions requiring ω_n to be orthogonal to polynomials of degree $k-1$. These are nonlinear constraints on the nodes τ_ν of (1.4.1). (If $k = 0$, there is no constraint, since $d = n-1$ is always attainable.) Once distinct nodes have been found that satisfy these constraints, the respective weights λ_ν, by (a), can be found by interpolation.

If $\mathrm{d}\lambda$ is a positive measure, then $k = n$ in Theorem 1.45 is optimal. Indeed, $k = n+1$, according to (b), would require orthogonality of ω_n to all polynomials of degree $\leq n$, in particular orthogonality onto itself. This is impossible. The optimal quadrature rule (1.4.1) with $k = n$, that is, having degree of exactness $d = 2n-1$, is called the *Gauss quadrature rule* with respect to the measure $\mathrm{d}\lambda$. Condition (b) then shows that $\omega_n(t) = \pi_n(t; \mathrm{d}\lambda)$, that is, the nodes τ_ν are the zeros of the polynomial of degree n orthogonal with respect to the measure $\mathrm{d}\lambda$. The weights λ_ν can be obtained by interpolation and, therefore, are also expressible in terms of orthogonal polynomials. Computationally, however, there are better ways to generate Gauss formulae (cf. §3.1.1).

1.4.2 *Gauss-type quadrature rules*

We assume in this subsection that the measure $\mathrm{d}\lambda$ is positive. The n-point Gauss quadrature rule will be written in the form

$$\int_{\mathbb{R}} f(t)\,\mathrm{d}\lambda(t) = \sum_{\nu=1}^{n} \lambda_\nu^G f(\tau_\nu^G) + R_n^G(f), \quad R_n^G(\mathbb{P}_{2n-1}) = 0, \tag{1.4.7}$$

where in the notation for the nodes and weights their dependence on n is suppressed. This formula, apart from being optimal with respect to degree of exactness, has a number of other remarkable properties.

Theorem 1.46 *All nodes $\tau_\nu = \tau_\nu^G$ are mutually distinct and contained in the interior of the support interval $[a,b]$ of $\mathrm{d}\lambda$, and all weights $\lambda_\nu = \lambda_\nu^G$ are positive.*

Proof Since τ_ν are the zeros of $\pi_n(\,\cdot\,;\mathrm{d}\lambda)$ (cf. the last paragraph of §1.4.1), the first assertion follows from Theorem 1.19. While formula (1.4.5) for λ_ν gives no clue as to their signs, it was Stieltjes who observed that

$$0 < \int_{\mathbb{R}} \ell_\mu^2(t)\,\mathrm{d}\lambda(t) = \sum_{\nu=1}^{n} \lambda_\nu \ell_\mu^2(\tau_\nu) = \lambda_\mu, \quad \mu = 1,2,\ldots,n,$$

where the first equality follows from the fact that $\ell_\mu^2 \in \mathbb{P}_{2n-2} \subset \mathbb{P}_{2n-1}$. □

Theorem 1.47 *The weights λ_ν^G are the coefficients in the partial fraction decomposition of σ_n/π_n* (cf. (1.3.33)),

$$\frac{\sigma_n(z)}{\pi_n(z)} = \sum_{\nu=1}^{n} \frac{\lambda_\nu^G}{z - \tau_\nu^G}\,. \tag{1.4.8}$$

In particular,

$$\lambda_\nu^G = \frac{\sigma_n(\tau_\nu^G)}{\pi_n'(\tau_\nu^G)}\,, \quad \nu = 1,2,\ldots,n. \tag{1.4.9}$$

Proof If, for the moment, we denote the partial fraction coefficients by λ_ν, we have from (1.3.43)

$$\int_{\mathbb{R}} \frac{\mathrm{d}\lambda(t)}{z-t} - \sum_{\nu=1}^{n} \frac{\lambda_\nu}{z - \tau_\nu^G} = O(z^{-2n-1}) \quad \text{as } z \to \infty.$$

By expanding both terms on the left in descending powers of z, we find that

$$\int_{\mathbb{R}} t^k\,d\lambda(t) - \sum_{\nu=1}^{n} \lambda_\nu [\tau_\nu^G]^k = 0, \quad k = 0,1,\ldots,2n-1.$$

This implies $\lambda_\nu = \lambda_\nu^G$. Multiplying (1.4.8) by $z - \tau_\nu^G$ and letting $z \to \tau_\nu^G$ yields (1.4.9). □

Theorem 1.48 (Markov) *There holds*

$$\sum_{\nu=1}^{n} \lambda_\nu^G f(\tau_\nu^G) = \int_{\mathbb{R}} p_{2n-1}(f;t)\,\mathrm{d}\lambda(t), \tag{1.4.10}$$

where $p_{2n-1}(f;\,\cdot\,)$ is the Hermite interpolation polynomial of degree $2n-1$ satisfying

$$p_{2n-1}(f;\tau_\nu^G) = f(\tau_\nu^G), \quad p_{2n-1}'(f;\tau_\nu^G) = f'(\tau_\nu^G), \quad \nu = 1,2,\ldots,n. \tag{1.4.11}$$

Proof As is well known, writing $\tau_\nu = \tau_\nu^G$, one has

$$p_{2n-1}(f;t) = \sum_{\nu=1}^{n} [h_\nu(t) f(\tau_\nu) + k_\nu(t) f'(\tau_\nu)], \tag{1.4.12}$$

where, with ℓ_ν as defined in (1.4.4),

$$\begin{aligned} h_\nu(t) &= (1 - 2(t-\tau_\nu)\ell_\nu'(\tau_\nu))\ell_\nu^2(t), \\ k_\nu(t) &= (t-\tau_\nu)\ell_\nu^2(t). \end{aligned} \tag{1.4.13}$$

Since h_ν, $k_\nu \in \mathbb{P}_{2n-1}$, there follows

$$\int_{\mathbb{R}} p_{2n-1}(f;t)\,\mathrm{d}\lambda(t) = \sum_{\nu=1}^{n} [\chi_\nu f(\tau_\nu) + \kappa_\nu f'(\tau_\nu)],$$

where

$$\begin{aligned} \chi_\nu &= \int_{\mathbb{R}} h_\nu(t)\,\mathrm{d}\lambda(t) = \sum_{\mu=1}^{n} \lambda_\mu (1 - 2(\tau_\mu - \tau_\nu)\ell_\nu'(\tau_\nu))\ell_\nu^2(\tau_\mu) = \lambda_\nu, \\ \kappa_\nu &= \int_{\mathbb{R}} k_\nu(t)\,\mathrm{d}\lambda(t) = \sum_{\mu=1}^{n} \lambda_\mu (\tau_\mu - \tau_\nu)\ell_\nu^2(\tau_\mu) = 0. \end{aligned}$$

□

Corollary to Theorem 1.48 If $f \in C^{2n}$ on the support interval $[a,b]$ of $\mathrm{d}\lambda$, then the remainder $R_n^G(f)$ in the Gauss formula (1.4.7) can be expressed as

$$R_n^G(f) = \frac{f^{(2n)}(\tau)}{(2n)!} \int_{\mathbb{R}} [\pi_n(t;\mathrm{d}\lambda)]^2\,\mathrm{d}\lambda(t), \quad \tau \in (a,b). \tag{1.4.14}$$

Proof For functions f satisfying the assumption of the corollary, it is well known from the theory of interpolation that

$$f(t) = p_{2n-1}(f;t) + r_{2n-1}(f;t), \tag{1.4.15}$$

where

$$r_{2n-1}(f;t) = \frac{f^{(2n)}(\tau(t))}{(2n)!} \prod_{\nu=1}^{n} (t-\tau_\nu)^2 \tag{1.4.16}$$

and $\tau(t) \in (a,b)$. Integrating (1.4.15) and using (1.4.16), (1.4.10), and (1.4.7) gives

$$R_n^G(f) = \int_{\mathbb{R}} r_{2n-1}(f;t)\,\mathrm{d}\lambda(t) = \int_{\mathbb{R}} \frac{f^{(2n)}(\tau(t))}{(2n)!} \prod_{\nu=1}^{n} (t-\tau_\nu)^2\,\mathrm{d}\lambda(t).$$

It now suffices to apply the mean value theorem of integration and to note that $\tau_\nu = \tau_\nu^G$ in order to obtain (1.4.14). □

Example 1.49 *Gauss–Chebyshev quadrature.*

This is (1.4.7) with $\mathrm{d}\lambda(t) = (1-t^2)^{-1/2}\,\mathrm{d}t$, the Chebyshev measure of the first kind (cf. Table 1.1). The nodes $\tau_\nu = \tau_\nu^G$ are the zeros of the Chebyshev polynomial T_n. Since $T_n(\cos\theta) = \cos n\theta$ (cf. (1.5.2)), one has

$$\tau_\nu = \cos\theta_\nu, \quad \theta_\nu = \frac{2\nu-1}{2n}\,\pi, \quad \nu = 1, 2, \ldots, n. \tag{1.4.17}$$

In order to find the weights $\lambda_\nu = \lambda_\nu^G$, we note that (1.4.7), being interpolatory, must be exact for $f(t) = T_k(t)$, $k = 0, 1, \ldots, n-1$. In view of (1.4.17) and the orthogonality of the Chebyshev polynomials, this can be written in the form

$$\sum_{\nu=1}^{n} \lambda_\nu \cos k\theta_\nu = \pi\delta_{k,0}, \quad k = 0, 1, \ldots, n-1. \tag{1.4.18}$$

An elementary computation (using Euler's formula for the cosine) will show that

$$\sum_{k=0}^{n-1}{}' \cos k\theta_\nu \cos k\theta_\mu = \tfrac{1}{2}\, n\delta_{\nu,\mu}, \quad \nu, \mu = 1, 2, \ldots, n, \tag{1.4.19}$$

where the prime means that the first term (for $k = 0$) is to be halved. Multiplying both sides of (1.4.18) by $\cos k\theta_\mu$ and then summing over k as in (1.4.19) yields $\frac{1}{2}\, n\lambda_\mu = \frac{1}{2}\,\pi$, that is, $\lambda_\mu = \pi/n$. Thus,

$$\int_{-1}^{1} f(t)(1-t^2)^{-1/2}\,\mathrm{d}t = \frac{\pi}{n}\sum_{\nu=1}^{n} f\left(\cos\frac{2\nu-1}{2n}\,\pi\right) + R_n^C(f). \tag{1.4.20}$$

We see that for each $n = 1, 2, 3, \ldots$, the n-point Gauss–Chebyshev quadrature rule has equal weights. According to a result of Posse (1875), this is the only Gauss quadrature rule that has this property.

If the support interval $[a, b]$ of $\mathrm{d}\lambda$ is bounded from below, that is, $a > -\infty$ and $b \le \infty$, it is sometimes convenient to have a quadrature rule in which one of the nodes is a, say $\tau_0 = a$. If, then, we replace n by $n+1$ in (1.4.1) and write $\omega_{n+1}(t) = (t-a)\omega_n(t)$, the optimal formula according to Theorem 1.45 requires ω_n to satisfy

$$\int_{\mathbb{R}} \omega_n(t)p(t)(t-a)\,\mathrm{d}\lambda(t) = 0 \quad \text{for } p \in \mathbb{P}_{n-1},$$

that is, $\omega_n(t) = \pi_n(t; \mathrm{d}\lambda_a)$, where $\mathrm{d}\lambda_a(t) = (t-a)\,\mathrm{d}\lambda(t)$. The remaining n nodes, therefore, must be the zeros of $\pi_n(\,\cdot\,; \mathrm{d}\lambda_a)$. The resulting $(n+1)$-point quadrature rule

$$\begin{gathered}\int_{\mathbb{R}} f(t)\,\mathrm{d}\lambda(t) = \lambda_0^a f(\tau_0^a) + \sum_{\nu=1}^{n} \lambda_\nu^a f(\tau_\nu^a) + R_n^a(f), \\ \tau_0^a = a, \quad \pi_n(\tau_\nu^a; \mathrm{d}\lambda_a) = 0, \quad \nu = 1, 2, \ldots, n,\end{gathered} \tag{1.4.21}$$

is called the *Gauss–Radau rule*. Similarly, if b also is bounded, $b < \infty$, and one wants both a and b to be nodes, one obtains the $(n+2)$-point *Gauss–Lobatto rule*

$$\begin{aligned} \int_a^b f(t)\,\mathrm{d}\lambda(t) &= \lambda_0^L f(\tau_0^L) + \sum_{\nu=1}^{n} \lambda_\nu^L f(\tau_\nu^L) + \lambda_{n+1}^L f(\tau_{n+1}^L) + R_n^{a,b}(f), \\ \tau_0^L = a, \quad \tau_{n+1}^L &= b, \quad \pi_n(\tau_\nu^L; \mathrm{d}\lambda_{a,b}) = 0, \quad \nu = 1, 2, \ldots, n, \end{aligned} \tag{1.4.22}$$

where now $\mathrm{d}\lambda_{a,b}(t) = (t-a)(b-t)\,\mathrm{d}\lambda(t)$. In (1.4.21), one has

$$R_n^a(f) = \gamma_n^a \frac{f^{(2n+1)}(\tau^a)}{(2n+1)!}, \quad \gamma_n^a = \int_{\mathbb{R}} [\pi_n(t; \mathrm{d}\lambda_a)]^2\, d\lambda_a(t), \tag{1.4.23}$$

while in (1.4.22) there holds

$$R_n^{a,b}(f) = -\gamma_n \frac{f^{(2n+2)}(\tau)}{(2n+2)!}, \quad \gamma_n = \int_a^b [\pi_n(t; \mathrm{d}\lambda_{a,b})]^2\, \mathrm{d}\lambda_{a,b}(t). \tag{1.4.24}$$

(The minus sign in (1.4.24) comes from changing the factor $(t-a)(t-b)$ in the node polynomial to $(t-a)(b-t)$ to make it, and with it, $\mathrm{d}\lambda_{a,b}(t) = (t-a)(b-t)\,\mathrm{d}\lambda(t)$, positive on $[a,b]$.) The two quadrature rules, therefore, have degrees of exactness respectively equal to $d^R = 2n$ and $d^L = 2n+1$. Both formulae remain valid if one takes $\tau_0^a < a$ resp. $\tau_0^L < a$ and/or $\tau_{n+1}^L > b$.

Example 1.50 Gauss–Lobatto formula for the Chebyshev measure $\mathrm{d}\lambda(t) = (1-t^2)^{-1/2}\,\mathrm{d}t$.

With $\tau_0^L = -1$, $\tau_{n+1}^L = 1$ in (1.4.22), the internal nodes τ_ν^L are the zeros of the polynomial of degree n orthogonal with respect to the measure $(1-t^2)\,\mathrm{d}\lambda(t) = (1-t^2)^{1/2}\,\mathrm{d}t$, that is, the Chebyshev polynomial U_n of the second kind (cf. Commentary to Table 1.1). Thus, $\tau_\nu^L = \cos((n+1-\nu)\pi/(n+1))$, $\nu = 1, 2, \ldots, n$. Moreover, known explicit formulae for the weights (see, e.g. Gautschi (2000b)) yield $\lambda_0^L = \lambda_{n+1}^L = \pi/(2n+2)$ and $\lambda_\nu^L = \pi/(n+1)$, $\nu = 1, 2, \ldots, n$. The Gauss–Lobatto formula in this case, therefore, is

$$\begin{aligned} \int_{-1}^{1} f(t)(1-t^2)^{-1/2}\,\mathrm{d}t = &\frac{\pi}{2(n+1)}\,[f(-1) + f(1)] \\ &+ \frac{\pi}{n+1} \sum_{\nu=1}^{n} f\left(\cos\frac{n+1-\nu}{n+1}\,\pi\right) + R_n^{\pm 1}(f) \end{aligned} \tag{1.4.25}$$

and has the distinguishing feature of having the same constant weight multiplying all internal terms and half that weight multiplying the boundary terms.

1.5 Classical orthogonal polynomials

There is no generally accepted definition of classical orthogonal polynomials, but loosely speaking they are those satisfying a linear second-order differential

or difference equation and possessing a Rodrigues-type formula. Jacobi polynomials and their special cases, and Laguerre, Hermite, and Meixner–Pollaczek polynomials, are probably the most widely used classical orthogonal polynomials of a continuous variable, and are certainly those most extensively studied. For their theory, Szegö (1975) is still the best source. Among the classical orthogonal polynomials of a discrete variable, the best known are those of Chebyshev, Krawtchouk, Charlier, Meixner, and Hahn. Some of the classical orthogonal polynomials, notably Chebyshev polynomials of the first two kinds, are of considerable importance for purposes of approximation. From the perspective of numerical computation, however, classical orthogonal polynomials are of marginal interest only, as their computation from the three-term recurrence relation is straightforward. Nevertheless, having recursion coefficients α_k, β_k that are known explicitly, they are useful in defining modified moments, which in turn often allows us to generate in a stable manner nonclassical orthogonal polynomials close, in some sense, to classical ones (cf. §2.1.7).

We limit ourselves, therefore, to providing in tabular form (Tables 1.1 and 1.2) a summary of the most commonly used classical orthogonal polynomials and their recursion coefficients, both for absolutely continuous and discrete measures. This will be supplemented by appropriate commentary.

1.5.1 *Classical orthogonal polynomials of a continuous variable*

Commentary to Table 1.1 Classical orthogonal polynomials, as conventionally used, are neither monic nor orthonormal, but are normalized in some *ad hoc* fashion. We comment on the normalizations in use and the notations that go with them. We also identify the leading coefficients k_n and squared norms h_n, that is,

$$p_n(t) = k_n t^n + \cdots, \quad h_n = \|p_n\|^2, \tag{1.5.1}$$

where p_n is the respective orthogonal polynomial of degree n. Where appropriate, some special extremal properties of interest in applications are included. The `OPQ` Matlab routines for generating the recurrence coefficients of the monic orthogonal polynomials are also referenced.

Legendre polynomials

The usual notation for the nth-degree Legendre polynomial is P_n and corresponds to the normalization $P_n(1) = 1$. One has $k_n = (2n)!/(2^n n!^2)$ and $h_n = 1/(n+\frac{1}{2})$. In terms of the P_n, the recurrence relation is

$$(k+1)P_{k+1}(t) = (2k+1)tP_k(t) - kP_{k-1}(t), \quad P_0(t) = 1,\ P_1(t) = t.$$

Each P_n is bounded by 1 on $[-1, 1]$. The shifted Legendre polynomials are denoted by P_n^*; one has $P_n^*(t) = P_n(2t-1)$. Matlab routines: `r_jacobi.m`, `r_jacobi01.m`.

Chebyshev polynomials

The Chebyshev polynomials of the *first kind*, T_n, are defined by

$$T_n(\cos\theta) = \cos n\theta, \tag{1.5.2}$$

so that $T_n(1) = 1$. One has $k_0 = 1$, $k_n = 2^{n-1}$ $(n \geq 1)$ and $h_0 = \pi$, $h_n = \frac{1}{2}\pi$ $(n \geq 1)$. Evidently, $|T_n| \leq 1$ on $[-1, 1]$.

The importance of the Chebyshev polynomials T_n in approximation stems from the extremal property in the uniform norm $\|u\|_\infty = \max_{-1\leq t\leq 1} |u(t)|$ satisfied by the monic Chebyshev polynomial $T_n^\circ = 2^{1-n}T_n$, $n \geq 1$,

$$\|p\|_\infty \geq \|T_n^\circ\|_\infty = 2^{1-n} \quad \text{for all } p \in \mathbb{P}_n^\circ. \tag{1.5.3}$$

Here, $\mathbb{P}_n^\circ$ is the class of monic polynomials of degree n. Equality in (1.5.3) holds if and only if $p = T_n^\circ$. It is also true that for any $a > 1$

$$\|p\|_\infty \geq \left\| \frac{T_n}{T_n(a)} \right\|_\infty \quad \text{for all } p \in \mathbb{P}_n(a) := \{p \in \mathbb{P}_n : \ p(a) = 1\}, \tag{1.5.4}$$

with equality holding if and only if $p = T_n/T_n(a)$. The norm is the same as in (1.5.3).

The Chebyshev polynomial of the *second kind*, U_n, is defined by

$$U_n(\cos\theta) = \frac{\sin(n+1)\theta}{\sin\theta}, \tag{1.5.5}$$

so that $U_n(1) = n + 1$. One has $k_n = 2^n$ and $h_n = \frac{1}{2}\pi$. The monic polynomial $U_n^\circ = 2^{-n}U_n$ also satisfies an extremal property, but this time in the L_1-norm $\|u\|_1 = \int_{-1}^1 |u(t)|\,\mathrm{d}t$,

$$\|p\|_1 \geq \|U_n^\circ\|_1 \quad \text{for all } p \in \mathbb{P}_n^\circ, \tag{1.5.6}$$

with equality if and only if $p = U_n^\circ$.

The Chebyshev polynomials V_n, W_n of the *third* and *fourth kinds* are defined, respectively, by

$$V_n(\cos\theta) = \frac{\cos(n+\frac{1}{2})\theta}{\cos\frac{1}{2}\theta}, \quad W_n(\cos\theta) = \frac{\sin(n+\frac{1}{2})\theta}{\sin\frac{1}{2}\theta} \tag{1.5.7}$$

and are normalized by $V_n(1) = 1$, $W_n(1) = 2n + 1$. Replacing θ by $\theta + \pi$ yields $W_n(t) = (-1)^n V_n(-t)$. One has $k_n = 2^n$ and $h_n = \pi$ for both U_n and V_n.

All four Chebyshev polynomials satisfy the same recurrence relation

$$y_{k+1} = 2ty_k - y_{k-1}, \quad k = 1, 2, \ldots, \tag{1.5.8}$$

where

$$y_0 = 1 \quad \text{and} \quad y_1 = \begin{cases} t & \text{for } T_n(t), \\ 2t & \text{for } U_n(T), \\ 2t-1 & \text{for } V_n(t), \\ 2t+1 & \text{for } W_n(t). \end{cases}$$

Matlab routine: `r_jacobi.m`.

Table 1.1 *Recurrence coefficients for classical monic orthogonal polynomials with respect to* $\mathrm{d}\lambda(t) = w(t)\,\mathrm{d}t$.

$w(t)$	Support	Name	α_k	β_0	β_k, $k \geq 1$
1	$[-1,1]$	Legendre	0	2	$1/(4-k^{-2})$
1	$[0,1]$	Shifted Legendre	$\frac{1}{2}$	1	$1/(4(4-k^{-2}))$
$(1-t^2)^{-1/2}$	$[-1,1]$	Chebyshev #1	0	π	$\frac{1}{2}$ $(k=1)$, $\frac{1}{4}$ $(k>1)$
$(1-t^2)^{1/2}$	$[-1,1]$	Chebyshev #2	0	$\frac{1}{2}\pi$	$\frac{1}{4}$
$(1-t)^{-1/2}(1+t)^{1/2}$	$[-1,1]$	Chebyshev #3	$\frac{1}{2}$ $(k=0)$ 0 $(k>0)$	π	$\frac{1}{4}$
$(1-t)^{1/2}(1+t)^{-1/2}$	$[-1,1]$	Chebyshev #4	$-\frac{1}{2}$ $(k=0)$ 0 $(k>0)$	π	$\frac{1}{4}$
$(1-t^2)^{\lambda-1/2}$, $\lambda > -\frac{1}{2}$	$[-1,1]$	Gegenbauer	0	$\sqrt{\pi}\,\frac{\Gamma(\lambda+\frac{1}{2})}{\Gamma(\lambda+1)}$	$\frac{k(k+2\lambda-1)}{4(k+\lambda)(k+\lambda-1)}$
$(1-t)^{\alpha}(1+t)^{\beta}$	$[-1,1]$				
$\alpha > -1$, $\beta > -1$		Jacobi	α_k^J	β_0^J	β_k^J
e^{-t}	$[0,\infty]$	Laguerre	$2k+1$	1	k^2
$t^{\alpha}\mathrm{e}^{-t}$, $\alpha > -1$	$[0,\infty]$	Generalized Laguerre	$2k+\alpha+1$	$\Gamma(1+\alpha)$	$k(k+\alpha)$
e^{-t^2}	$[-\infty,\infty]$	Hermite	0	$\sqrt{\pi}$	$\frac{1}{2}k$
$\lvert t\rvert^{2\mu}\mathrm{e}^{-t^2}$, $\mu > -\frac{1}{2}$	$[-\infty,\infty]$	Generalized Hermite	0	$\Gamma(\mu+\frac{1}{2})$	$\frac{1}{2}k$ (k even) $\frac{1}{2}k+\mu$ (k odd)
$\frac{1}{2\pi}\mathrm{e}^{(2\phi-\pi)t}\lvert\Gamma(\lambda+it)\rvert^2$	$[-\infty,\infty]$	Meixner–Pollaczek	$-\frac{k+\lambda}{\tan\phi}$	$\frac{\Gamma(2\lambda)}{(2\sin\phi)^{2\lambda}}$	$\frac{k(k+2\lambda-1)}{4\sin^2\phi}$
$\lambda > 0$, $0 < \phi < \pi$					

$$\alpha_k^J = \frac{\beta^2-\alpha^2}{(2k+\alpha+\beta)(2k+\alpha+\beta+2)}{}^{*}$$
$$\beta_0^J = \frac{2^{\alpha+\beta+1}\Gamma(\alpha+1)\Gamma(\beta+1)}{\Gamma(\alpha+\beta+1)},\ \beta_k^J = \frac{4k(k+\alpha)(k+\beta)(k+\alpha+\beta)}{(2k+\alpha+\beta)^2(2k+\alpha+\beta+1)(2k+\alpha+\beta-1)}{}^{\dagger}$$

*If $k=0$, the common factor $\alpha+\beta$ in the numerator and denominator of α_0^J should be (must be, if $\alpha+\beta=0$) cancelled.
†If $k=1$, the last factors in the numerator and denominator of β_1^J should be (must be, if $\alpha+\beta+1=0$) cancelled.

Gegenbauer polynomials

These are customarily defined in terms of Jacobi polynomials $P_n^{(\alpha,\beta)}$ (see below) by

$$P_n^{(\lambda)}(t) = \frac{\Gamma(\lambda+\frac{1}{2})}{\Gamma(2\lambda)}\,\frac{\Gamma(n+2\lambda)}{\Gamma(n+\lambda+\frac{1}{2})}\,P_n^{(\lambda-\frac{1}{2},\lambda-\frac{1}{2})}(t) \quad \text{if } \lambda \neq 0.$$

Special cases are $P_n^{(1/2)} = P_n$ and $P_n^{(1)} = U_n$. Note that $P_0^{(\lambda)} = 1$, also as $\lambda \to 0$. If $n \geq 1$, however, $P_n^{(0)} \equiv 0$, but

$$\lim_{\lambda\to 0} \frac{P_n^{(\lambda)}(t)}{\lambda} = \frac{2}{n}\,T_n(t), \quad n \geq 1.$$

For $\lambda \neq 0$, one has $P_n^{(\lambda)}(1) = \binom{n+2\lambda-1}{n}$, $n \geq 1$, and

$$k_n = \frac{2^n}{n!}\,\frac{\Gamma(n+\lambda)}{\Gamma(\lambda)}, \quad h_n = \frac{2^{1-2\lambda}\Gamma(n+2\lambda)}{n!(n+\lambda)\Gamma^2(\lambda)}\,\pi.$$

The three-term recurrence relation for the $P_n^{(\lambda)}$, $\lambda \neq 0$, is

$$(k+1)P_{k+1}^{(\lambda)}(t) = 2(k+\lambda)tP_k^{(\lambda)}(t) - (k+2\lambda-1)P_{k-1}^{(\lambda)}(t),$$
$$k = 1, 2, 3, \ldots,$$
$$P_0^{(\lambda)}(t) = 1, \quad P_1^{(\lambda)}(t) = 2\lambda t.$$

In the limit $\lambda \to 0$, after division of $P_n^{(\lambda)}$, $n \geq 1$, by λ, it becomes the recurrence relation for the Chebyshev polynomials T_n. Matlab routine: `r_jacobi.m`.

Jacobi polynomials

The standard notation for the Jacobi polynomial of degree n is $P_n^{(\alpha,\beta)}$. It is normalized by $P_n^{(\alpha,\beta)}(1) = \binom{n+\alpha}{n}$, giving

$$k_n = \frac{1}{2^n}\binom{2n+\alpha+\beta}{n}, \quad h_n = \frac{2^{\alpha+\beta+1}}{2n+\alpha+\beta+1}\,\frac{\Gamma(n+\alpha+1)\Gamma(n+\beta+1)}{n!\Gamma(n+\alpha+\beta+1)}.$$

The three-term recurrence relation then is

$$2(k+1)(k+\alpha+\beta+1)(2k+\alpha+\beta)P_{k+1}^{(\alpha,\beta)}(t)$$
$$= (2k+\alpha+\beta+1)[(2k+\alpha+\beta+2)(2k+\alpha+\beta)t + \alpha^2 - \beta^2]P_k^{(\alpha,\beta)}(t)$$
$$-2(k+\alpha)(k+\beta)(2k+\alpha+\beta+2)P_{k-1}^{(\alpha,\beta)}(t), \quad k = 1, 2, 3, \ldots,$$
$$P_0^{(\alpha,\beta)}(t) = 1, \quad P_1^{(\alpha,\beta)}(t) = \tfrac{1}{2}(\alpha+\beta+2)t + \tfrac{1}{2}(\alpha-\beta).$$

Interchanging the parameters α and β has the effect of reflecting the argument at the origin,

$$P_n^{(\beta,\alpha)}(t) = (-1)^n P_n^{(\alpha,\beta)}(-t).$$

Matlab routines: `r_jacobi.m`, `r_jacobi01.m`.

There are weight functions that are less conventional and yet have orthogonal polynomials expressible in terms of Jacobi polynomials. An example is $w(t) = |t|^\gamma(1-t^2)^\alpha$ on $[-1,1]$, where $\gamma > -1$ and $\alpha > -1$. The respective orthogonal polynomials of even degree are $P_{n/2}^{(\alpha,(\gamma-1)/2)}(2t^2-1)$, and those of odd degree $tP_{\lfloor n/2\rfloor}^{(\alpha,(\gamma+1)/2)}(2t^2-1)$ (see Szegö (1975, eqn (4.1.6)) for $\alpha = 0$ and Laščenov (1953) or Chihara (1978, p. 156) for general $\alpha > -1$).

Laguerre polynomials

The Laguerre and generalized Laguerre polynomials are usually denoted by $L_n = L_n^{(0)}$ resp. $L_n^{(\alpha)}$. They are normalized by $L_n^{(\alpha)}(0) = \binom{n+\alpha}{n}$ and satisfy

$$k_n = \frac{(-1)^n}{n!}, \quad h_n = \frac{\Gamma(\alpha+n+1)}{n!}.$$

Note that the leading coefficient k_n is alternately positive and negative, contrary to general convention. The three-term recurrence relation is

$$(k+1)L_{k+1}^{(\alpha)}(t) = (2k+\alpha+1-t)L_k^{(\alpha)}(t) - (k+\alpha)L_{k-1}^{(\alpha)}(t), \qquad k = 1,2,3,\ldots,$$
$$L_0^{(\alpha)}(t) = 1, \quad L_1^{(\alpha)}(t) = \alpha+1-t.$$

Matlab routine: `r_laguerre.m`. The following bounds are valid for $t \geq 0$,

$$\mathrm{e}^{-t/2}|L_n^{(\alpha)}(t)| \leq \begin{cases} 2 - \dfrac{\Gamma(\alpha+n+1)}{n!\Gamma(\alpha+1)} & \text{if } -1 < \alpha < 0, \\ \dfrac{\Gamma(\alpha+n+1)}{n!\Gamma(\alpha+1)} & \text{if } \alpha \geq 0. \end{cases}$$

Hermite polynomials

The Hermite polynomials H_n, as customarily defined, satisfy

$$k_n = 2^n, \quad h_n = \sqrt{\pi}\,2^n n!$$

and obey the three-term recurrence relation

$$H_{k+1}(t) = 2tH_k(t) - 2kH_{k-1}(t), \quad k = 1,2,3,\ldots,$$
$$H_0(t) = 1, \quad H_1(t) = 2t.$$

Matlab routine: `r_hermite.m`. The following bound holds for $t \in \mathbb{R}$,

$$\mathrm{e}^{-t^2/2}|H_n(t)| \leq \sqrt{2^n n!}.$$

The *generalized* Hermite polynomials $H_n^{(\mu)}$ are normalized by

$$k_n = 2^n, \quad h_n = 2^{2n}\,\Gamma\left(\left\lfloor \frac{n+2}{2} \right\rfloor\right)\left(\Gamma\left(\left\lfloor \frac{n+1}{2} \right\rfloor\right) + \mu + \frac{1}{2}\right).$$

They are related to generalized Laguerre polynomials via the formulae (Chihara, 1978, Chapter V, eqn (2.43))

$$2^{-n}H_n^{(\mu)}(t) = \begin{cases} \left(\frac{n}{2}\right)!\, L_{n/2}^{(\mu-1/2)}(t^2), & n \text{ even}, \\ -\left(\frac{n-1}{2}\right)!\, t L_{(n-1)/2}^{(\mu+1/2)}(t^2), & n \text{ odd}. \end{cases}$$

Meixner–Pollaczek polynomials

The Meixner–Pollaczek polynomial of degree n, denoted by $P_n^{(\lambda)}(t;\phi)$, has

$$k_n = \frac{(2\sin\phi)^n}{n!}, \quad h_n = \frac{\Gamma(n+2\lambda)}{(2\sin\phi)^{2\lambda} n!},$$

and satisfies the three-term recurrence relation

$$(k+1)P_{k+1}^{(\lambda)}(t;\phi) = 2[t\sin\phi + (k+\lambda)\cos\phi]P_k^{(\lambda)}(t;\phi) - (k+2\lambda-1)P_{k-1}^{(\lambda)}(t;\phi),$$
$$k = 1, 2, 3, \ldots,$$
$$P_0^{(\lambda)}(t;\phi) = 1, \quad P_1^{(\lambda)}(t;\phi) = 2(t\sin\phi + \lambda\cos\phi).$$

For $\phi = \frac{1}{2}\pi$, the polynomial $P_n^{(\lambda)}(t;\frac{1}{2}\pi)$ is even or odd depending on the parity of n. Matlab routine: `r_meixner_pollaczek.m`.

1.5.2 *Classical orthogonal polynomials of a discrete variable*

Commentary to Table 1.2 Notations vary in the literature; we follow the one used in the Appendix of Askey and Wilson (1985).

Discrete Chebyshev polynomials

These are the polynomials $t_n(\,\cdot\,) = t_n(\,\cdot\,;N)$ of Example 1.15. They satisfy

$$k_n = \frac{(2n)!}{n!^2}, \quad h_n = \frac{(N+n)!}{(2n+1)(N-n-1)!},$$

and obey the recurrence relation

$$(n+1)t_{n+1}(x) = 2(2n+1)(x - \tfrac{1}{2}(N-1))t_n(x) - n(N^2-n^2)t_{n-1}(x),$$
$$n = 0, 1, \ldots, N-1,$$
$$t_0(x) = 1, \quad t_1(x) = 2x - N + 1.$$

Matlab routine: `r_hahn.m`.

Table 1.2 *Recurrence coefficients for monic discrete orthogonal polynomials with respect to* $\mathrm{d}\lambda(x) = \sum_{k=0}^{M} w(x)\delta(x - x_k)\,\mathrm{d}x$.

$w(x_k)$	M	x_k	Name	α_n	β_0	$\beta_n,\ 1 \le n \le M$
1	$N-1$	k	Discrete Chebyshev	$\frac{N}{2}\left(1 - \frac{1}{N}\right)$	N	$\frac{N^2}{4}\,\frac{1-(n/N)^2}{4-1/n^2}$
$\binom{N}{k} p^k (1-p)^{N-k}$ $0 < p < 1$	N	k	Krawtchouk	$n + p(N-2n)$	1	$p(1-p)n(N-n+1)$
$\frac{\mathrm{e}^{-a} a^k}{k!}$, $a > 0$	∞	k	Charlier	$n + a$	1	an
$\frac{c^k}{\Gamma(\beta)}\,\frac{\Gamma(k+\beta)}{k!}$ $0 < c < 1,\ \beta > 0$	∞	k	Meixner	$\frac{(1+c)n + \beta c}{1-c}$	$(1-c)^{-\beta}$	$\frac{c}{(1-c)^2}\, n(n+\beta-1)$
$\binom{\alpha+k}{k}\binom{\beta+N-k}{N-k}$	N	k	Hahn	α_n^H	β_0^H	β_n^H

$\alpha_n^H = A_n + C_n$, $\beta_0^H = (\alpha+\beta+2)_N / N!$, $\beta_n^H = A_{n-1} C_n$ $(n \ge 1)$

$$A_n = \frac{(n+\alpha+\beta+1)(n+\alpha+1)(N-n)}{(2n+\alpha+\beta+1)(2n+\alpha+\beta+2)},\quad C_n = \frac{n(n+\alpha+\beta+N+1)(n+\beta)}{(2n+\alpha+\beta)(2n+\alpha+\beta+1)}$$

The choice $x_k = k$, $k = 0, 1, \ldots, N-1$, of the support points is a canonical one, corresponding to the interval $[0, N-1]$. A linear transformation of variables $t = a + (x/(N-1))(b-a)$ will map the points x_k to equally spaced points $t_k = a + (k/(N-1))(b-a)$ on the interval $[a, b]$. The corresponding monic orthogonal polynomials in the t-variable then satisfy the recurrence relation $\pi_{n+1}(t) = (t - a_n)\pi_n(t) - b_n\pi_{n-1}(t)$, $\pi_{-1}(t) = 0$, $\pi_0(t) = 1$, where

$$a_n = a + \frac{b-a}{N-1}\,\alpha_n, \quad b_n = \left(\frac{b-a}{N-1}\right)^2 \beta_n, \quad n = 1, 2, \ldots, N-1.$$

Thus, for example, if $a = 0$, $b = 1$, then $a_n = \frac{1}{2}$, $b_n = \frac{1}{4}(1 + (1/(N-1)))^2(1 - (n/N)^2)/(4 - 1/n^2)$, which for $N \to \infty$ tend to the recursion coefficients of the shifted Legendre polynomials (cf. Table 1.1).

Krawtchouk polynomials with parameter p

Krawtchouk polynomials are widely used in coding theory; see, for example, Bannai (1990). Denoted by $K_n(\,\cdot\,) = K_n(\,\cdot\,; p, N)$ and normalized by

$$k_n = \frac{1}{n!}, \quad h_n = \binom{N}{n}[p(1-p)]^n,$$

they satisfy the three-term recurrence relation

$$(n+1)K_{n+1}(x) = [x - (n + p(N-2n))]K_n(x) - (N-n+1)p(1-p)K_{n-1}(x), \qquad n = 0, 1, \ldots, N,$$

$$K_0(x) = 1, \quad K_1(x) = x - pN.$$

Charlier polynomials with parameter a

Charlier polynomials are used in statistics. Their notation is $C_n(\,\cdot\,) = C_n(\,\cdot\,; a)$ if normalized by

$$k_n = \frac{(-1)^n}{a^n}, \quad h_n = \frac{n!}{a^n}\,\mathrm{e}^a.$$

(Note again the unconventional sign of the leading coefficient.) The recurrence relation is

$$aC_{n+1}(x) = (n + a - x)C_n(x) - nC_{n-1}(x), \quad n = 0, 1, 2, \ldots,$$

$$C_0(x) = 1, \quad C_1(x) = -\frac{1}{a}\,x.$$

Meixner polynomials with parameters β, c

These are denoted by $M_n(\,\cdot\,) = M_n(\,\cdot\,;\beta,c)$ and satisfy

$$k_n = \frac{1}{(\beta)_n}\left(\frac{c-1}{c}\right)^n, \quad h_n = \frac{1}{(\beta)_n}\,\frac{n!}{c^n(1-c)^\beta}\ ,$$

where $(\beta)_n = \beta(\beta+1)\cdots(\beta+n-1)$. Their recurrence relation is

$$(n+\beta)cM_{n+1}(x) = [(c-1)x + (1+c)n + \beta c]M_n(x) - nM_{n-1}(x),$$
$$n = 0,1,2,\ldots,$$
$$M_0(x) = 1, \quad M_1(x) = \frac{c-1}{\beta c}\,x + 1.$$

The Charlier polynomials are a limit case of Meixner polynomials,

$$C_n(x;a) = \lim_{\beta\to\infty} M_n\left(x;\beta,\frac{a}{\beta+a}\right).$$

Hahn polynomials with parameters α, β

Here, the notation is $Q_n(\,\cdot\,) = Q_n(\,\cdot\,;\alpha,\beta,N)$, and the normalization

$$k_n = \frac{\Gamma(\alpha+1)\Gamma(2n+\alpha+1)}{\Gamma(n+\alpha+1)\Gamma(n+\alpha+\beta+1)},$$
$$h_n = \frac{\Gamma(\alpha+1)\Gamma(n+\beta+1)\Gamma(n+\alpha+\beta+N+2)n!}{(2n+\alpha+\beta+1)\Gamma(\beta+1)\Gamma(n+\alpha+1)\Gamma(n+\alpha+\beta+1)(N-n)!}\,.$$

The recurrence relation in Table 1.2, rewritten in terms of the Q_ns, becomes

$$\frac{k_{n+1}}{k_n}\,Q_{n+1}(x) = [x-(A_n+C_n)]Q_n(x) - \frac{k_n}{k_{n-1}}\,A_{n-1}C_nQ_{n-1}(x),$$
$$n = 0,1,\ldots,N,$$
$$Q_0(x) = 1, \quad Q_1(x) = 1 - \frac{\alpha+\beta+2}{(\alpha+1)N}\,x,$$

where A_n, C_n are as defined in Table 1.2. For $\alpha = \beta = 0$, the Hahn polynomials become the discrete Chebyshev polynomials,

$$Q_n(x;0,0,N) = t_n(x;N+1).$$

Matlab routine: `r_hahn.m`.

1.6 Kernel polynomials

In this section, the class of measures $\mathrm{d}\lambda$ is extended to include real or complex-valued measures on $\mathbb{R}$. The assumption of all moments (1.1.1) being finite, however, is maintained and will be tacitly made.

1.6.1 *Existence and elementary properties*

Definition 1.51 *A real or complex-valued measure* $\mathrm{d}\lambda$ *is said to be* quasi-definite *if all its Hankel determinants (1.1.5) are nonzero,*

$$\Delta_n = \det \boldsymbol{M}_n \neq 0, \quad n = 1, 2, 3, \dots \ . \tag{1.6.1}$$

A system of monic polynomials $\pi_0, \pi_1, \pi_2, \dots$ *is called* formal orthogonal *with respect to* $\mathrm{d}\lambda$ *if (1.1.8) holds with the positivity requirement replaced by* $\|\pi_k\|_{\mathrm{d}\lambda} \neq 0$ *for* $k = 0, 1, 2, \dots$.

Theorem 1.52 *There exists a unique system* $\pi_0, \pi_1, \pi_2 \dots$ *of monic formal orthogonal polynomials with respect to* $\mathrm{d}\lambda$ *if and only if* $\mathrm{d}\lambda$ *is quasi-definite.*

Proof Let $n \geq 1$ and $\pi_n(t) = t^n + a_{n-1}t^{n-1} + \cdots + a_0$. Orthogonality requires $(\pi_n, t^k) = 0$ for $k = 0, 1, \dots, n-1$, which is a system of linear equations for the vector $\boldsymbol{a}^{\mathrm{T}} = [a_0, a_1, \dots, a_{n-1}]$ with the coefficient matrix being $\boldsymbol{M}_n$. The system has a unique solution if and only if $\boldsymbol{M}_n$ is nonsingular. Since this must hold for each $n \geq 1$, quasi-definiteness is a necessary condition for the existence of formal orthogonal polynomials. The condition is also sufficient since $(\pi_n, \pi_n) = 0$ would imply $(\pi_n, t^n) = 0$, which, adjoined to the previous system, would yield

$$\boldsymbol{M}_{n+1} \begin{bmatrix} \boldsymbol{a} \\ 1 \end{bmatrix} = \boldsymbol{0}.$$

This contradicts nonsingularity of $\boldsymbol{M}_{n+1}$. Therefore, $(\pi_n, \pi_n) \neq 0$. □

All the properties of orthogonal polynomials that do not depend on positivity arguments continue to remain in force. This includes the symmetry properties of §1.2.1 and, more importantly, Theorem 1.27, guaranteeing the existence of a three-term recurrence relation. The coefficients $\alpha_k(\mathrm{d}\lambda)$ and $\beta_k(\mathrm{d}\lambda)$ in (1.3.2), however, are now in general real or complex numbers, and all we can say about β_k is that

$$\beta_k(\mathrm{d}\lambda) \neq 0, \quad k = 0, 1, 2, \dots \ . \tag{1.6.2}$$

(The case $k = 0$ follows from $\beta_0 = \Delta_1$ and $\Delta_1 \neq 0$.)

For an arbitrary $z \in \mathbb{C}$ let

$$\left.\begin{aligned} \alpha_k &= z + q_k + e_{k-1} \\ \beta_k &= e_{k-1} q_{k-1} \end{aligned}\right\} \ k = 0, 1, 2, \dots \ ; \ e_{-1} = q_{-1} = 0, \tag{1.6.3}$$

where $\alpha_k = \alpha_k(\mathrm{d}\lambda)$, $\beta_k = \beta_k(\mathrm{d}\lambda)$. The monic formal orthogonal polynomials are denoted, as before, by $\pi_k(\,\cdot\,) = \pi_k(\,\cdot\,; \mathrm{d}\lambda)$.

Lemma 1.53 *Let* $\mathrm{d}\lambda$ *be quasi-definite.*

(a) *If* $\pi_n(z) \neq 0$ *for* $n = 1, 2, 3, \ldots$, *then the relations (1.6.3) uniquely determine* $q_0, e_0, q_1, e_1, \ldots$ *in this order, and*

$$q_n = -\frac{\pi_{n+1}(z)}{\pi_n(z)}, \quad n = 0, 1, 2, \ldots . \tag{1.6.4}$$

(b) *If* $\pi_n(z) \neq 0$ *only for* $n \leq d$, *and* $\pi_{d+1}(z) = 0$, *then (1.6.4) holds for* $n < d$ *and* $q_d = 0$. *All* e_n *for* $n < d$ *are uniquely defined, but* e_d *remains undefined.*

Proof (a) The quantities $q_0, e_0, q_1, e_1, \ldots$ are uniquely defined if and only if in the process of generating the qs none of them vanishes. It suffices, therefore, to prove (1.6.4). We do this by induction on n. For $n = 0$, the first relation in (1.6.3) gives

$$q_0 = \alpha_0 - z = -(z - \alpha_0) = -\pi_1(z),$$

which by virtue of $\pi_0(z) = 1$ proves (1.6.4) for $n = 0$. Now assume (1.6.4) is true for $n = k - 1$, $k \geq 1$. Then by (1.6.3),

$$q_k = \alpha_k - z - e_{k-1} = \alpha_k - z - \frac{\beta_k}{q_{k-1}} = \alpha_k - z + \beta_k \frac{\pi_{k-1}(z)}{\pi_k(z)}.$$

Therefore,

$$q_k = -\frac{1}{\pi_k(z)} \left[(z - \alpha_k)\pi_k(z) - \beta_k \pi_{k-1}(z)\right] = -\frac{\pi_{k+1}(z)}{\pi_k(z)}$$

by (1.3.2) with t replaced by z. This is (1.6.4) for $n = k$.

(b) The argument used in (a) establishes (1.6.4) for $n \leq d$. In particular, $q_n \neq 0$ for $n < d$, implying that e_n for $n < d$ is well defined from the second relation in (1.6.3). On the other hand, $q_d = 0$, which leaves e_d undefined. □

Definition 1.54 *Let* $\mathrm{d}\lambda$ *be quasi-definite and* $\pi_k(\,\cdot\,) = \pi_k(\,\cdot\,; \mathrm{d}\lambda)$ *be the monic formal orthogonal polynomials with respect to* $\mathrm{d}\lambda$. *Let* $z \in \mathbb{C}$ *and assume that* $\pi_k(z) \neq 0$ *for* $k = 1, 2, 3, \ldots$. *Then,*

$$\hat{\pi}_n(t; z) = \frac{1}{t - z} \left[\pi_{n+1}(t) - \frac{\pi_{n+1}(z)}{\pi_n(z)} \pi_n(t)\right] \tag{1.6.5}$$

is called the kernel polynomial *for the measure* $\mathrm{d}\lambda$.

Evidently, $\hat{\pi}_n \in \mathbb{P}_n$. Since $\hat{\pi}_n(t; z) \sim t^n$ as $t \to \infty$, the kernel polynomial $\hat{\pi}_n$ is in fact a monic polynomial of degree n.

Theorem 1.55 *Let* $\mathrm{d}\lambda$ *be quasi-definite and* $z \in \mathbb{C}$ *be such that* $\pi_k(z) \neq 0$ *for* $k = 1, 2, 3 \ldots$. *Let* $\mathrm{d}\hat{\lambda}(t) = (t - z)\,\mathrm{d}\lambda(t)$. *Then,* $\mathrm{d}\hat{\lambda}$ *is also quasi-definite and the kernel polynomials* $\hat{\pi}_0, \hat{\pi}_1, \hat{\pi}_2, \ldots$ *are the monic formal orthogonal polynomials relative to* $\mathrm{d}\hat{\lambda}$.

Proof It suffices to prove the last statement of the theorem. Quasi-definiteness of $\mathrm{d}\hat{\lambda}$ then follows from Theorem 1.52.

By definition,

$$(\hat{\pi}_n, t^k)_{\mathrm{d}\hat{\lambda}} = (\pi_{n+1}, t^k)_{\mathrm{d}\lambda} - \frac{\pi_{n+1}(z)}{\pi_n(z)} (\pi_n, t^k)_{\mathrm{d}\lambda},$$

which is zero for $k < n$ and nonzero for $k = n$. □

Lemma 1.56 *Let the inner product for* $\mathrm{d}\lambda$ *be positive definite and assume* $\pi_n(z; \mathrm{d}\lambda) \neq 0$ *for* $n = 1, 2, 3, \ldots$. *Then, there holds*

(a) $\hat{\pi}_n(z; z) \neq 0$ *for* $n = 1, 2, 3, \ldots$ *if* $z \in \mathbb{R}$;

(b) $\hat{\pi}_n(\overline{z}; z) \neq 0$ *for* $n = 1, 2, 3, \ldots$ *if* $z \in \mathbb{C}$.

Proof (a) Taking the limit $t \to z$ in (1.6.5) gives

$$\hat{\pi}_n(z; z) = \frac{D_n(z)}{\pi_n(z)}, \quad D_n(z) := \pi_n(z)\pi'_{n+1}(z) - \pi_{n+1}(z)\pi'_n(z).$$

A simple calculation based on the recurrence relation (1.3.2) for π_k yields

$$D_{-1}(z) = 0, \quad D_n(z) = \pi_n^2(z) + \beta_n D_{n-1}(z), \quad n = 0, 1, 2, \ldots,$$

from which, in succession, $D_0(z) > 0, D_1(z) > 0, D_2(z) > 0, \ldots$, since z is real and $\beta_n > 0$ by assumption. Therefore, $\hat{\pi}_n(z; z) \neq 0$ for all n.

(b) If z is real, the assertion reduces to the one in (a). Assume, therefore, that $\operatorname{Im} z \neq 0$. Then,

$$\hat{\pi}_n(\overline{z}; z) = \frac{E_n(z)}{(\overline{z} - z)\pi_n(z)}, \quad E_n(z) := \pi_n(z)\pi_{n+1}(\overline{z}) - \pi_{n+1}(z)\pi_n(\overline{z}).$$

Since π_k are real polynomials,

$$E_n(z) = \pi_n(z)\overline{\pi_{n+1}(z)} - \pi_{n+1}(z)\overline{\pi_n(z)} = 2\mathrm{i}\operatorname{Im}\{\pi_n(z)\overline{\pi_{n+1}(z)}\}.$$

With $z = x + \mathrm{i}y$ and $v_n = \operatorname{Im}\{\pi_n(z)\overline{\pi_{n+1}(z)}\}$, the recurrence relation (1.3.2) again yields

$$v_{-1} = 0, \quad v_n = -y|\pi_n(z)|^2 + \beta_n v_{n-1}, \quad n = 0, 1, 2, \ldots,$$

hence, in succession, $\operatorname{sgn}(v_n) = -\operatorname{sgn}(y)$ for $n = 0, 1, 2, \ldots$, and $E_n(z) \neq 0$ for all n, so that $\hat{\pi}_n(\overline{z}; z) \neq 0$ for all n. □

1.6.2 *Recurrence relation*

Let $\hat{\alpha}_k$ and $\hat{\beta}_k$ be the recursion coefficients for the kernel polynomials $\hat{\pi}_n(\,\cdot\,) = \hat{\pi}_n(\,\cdot\,; z)$ in (1.6.5),

$$\begin{gathered} \hat{\pi}_{k+1}(t) = (t - \hat{\alpha}_k)\hat{\pi}_k(t) - \hat{\beta}_k\hat{\pi}_{k-1}(t), \quad k = 0, 1, 2, \ldots, \\ \hat{\pi}_{-1}(t) = 0, \quad \hat{\pi}_0(t) = 1. \end{gathered} \tag{1.6.6}$$

The following theorem shows how the coefficients $\hat{\alpha}_k$ and $\hat{\beta}_k$ can be generated in terms of the quantities q_k and e_k of Lemma 1.53.

Theorem 1.57 *Let* $\mathrm{d}\lambda$ *be quasi-definite and* $z \in \mathbb{C}$ *be such that* $\pi_n(z; \mathrm{d}\lambda) \neq 0$ *for all* n. *Let* q_k *and* e_k *be the quantities uniquely determined by (1.6.3). Then,*

$$\left.\begin{aligned} \hat{\alpha}_k &= z + q_k + e_k \\ \hat{\beta}_k &= q_k e_{k-1} \end{aligned}\right\} \quad k = 0, 1, 2, \dots \ . \tag{1.6.7}$$

Remarks to Theorem 1.57 1. In (1.6.7), $\hat{\beta}_0$ is set equal to zero; it could be assigned any other convenient value, such as $\hat{\beta}_0 = \int_{\mathbb{R}} \mathrm{d}\hat{\lambda}(t)$.

2. For computational purposes, it is better to write the first relation in (1.6.7), using (1.6.3), in the form

$$\hat{\alpha}_k = \alpha_k - e_{k-1} + e_k.$$

The reason is that, by (1.6.4), when $|z| > 1$,

$$q_k = -\frac{\pi_{k+1}(z)}{\pi_k(z)} \sim -z \quad \text{for } k \to \infty,$$

so that the term $z + q_k$ in (1.6.7) is subject to cancellation error. Depending on the magnitude of e_k, this could be detrimental to the relative accuray of $\hat{\alpha}_k$.

Proof By (1.6.5) and (1.6.4), one has

$$\hat{\pi}_k(t) = \frac{1}{t - z} \left[\pi_{k+1}(t) + q_k \pi_k(t)\right], \tag{1.6.8}$$

hence

$$\pi_{k+1}(t) = (t - z)\hat{\pi}_k(t) - q_k \pi_k(t), \quad k = 0, 1, 2, \dots \ . \tag{1.6.9}$$

Substituting (1.6.3) into the recurrence relation for π_k gives

$$\pi_{k+1}(t) = (t - z)\pi_k(t) - (q_k + e_{k-1})\pi_k(t) - e_{k-1} q_{k-1} \pi_{k-1}(t),$$

from which

$$\frac{\pi_{k+1}(t) + q_k \pi_k(t)}{t - z} = \pi_k(t) - e_{k-1} \frac{\pi_k(t) + q_{k-1}\pi_{k-1}(t)}{t - z},$$

or, by (1.6.8),

$$\hat{\pi}_k(t) = \pi_k(t) - e_{k-1}\hat{\pi}_{k-1}(t), \quad k = 0, 1, 2, \dots \ . \tag{1.6.10}$$

Replacing k by $k + 1$ in (1.6.10), and applying first (1.6.9), and then again (1.6.10), yields

$$\begin{aligned} \hat{\pi}_{k+1}(t) &= \pi_{k+1}(t) - e_k \hat{\pi}_k(t) \\ &= (t - z)\hat{\pi}_k(t) - q_k \pi_k(t) - e_k \hat{\pi}_k(t) \\ &= (t - z)\hat{\pi}_k(t) - q_k[\hat{\pi}_k(t) + e_{k-1}\hat{\pi}_{k-1}(t)] - e_k \hat{\pi}_k(t), \end{aligned}$$

that is,

$$\hat{\pi}_{k+1}(t) = (t - z - q_k - e_k)\hat{\pi}_k(t) - q_k e_{k-1}\hat{\pi}_{k-1}(t), \quad k = 0, 1, 2, \dots . \tag{1.6.11}$$

The assertion (1.6.7) now follows immediately by comparing (1.6.11) with (1.6.6). □

Theorem 1.57 is closely related to the QD algorithm of Rutishauser (Rutishauser, 1957; Stiefel, 1958). Indeed, if in analogy to (1.6.3) one writes

$$\left.\begin{aligned} \hat{\alpha}_k &= z + \hat{q}_k + \hat{e}_{k-1} \\ \hat{\beta}_k &= \hat{e}_{k-1}\hat{q}_{k-1} \end{aligned}\right\} \; k = 0, 1, 2, \dots ; \; \hat{e}_{-1} = \hat{q}_{-1} = 0,$$

then (1.6.7) immediately yields the "rhombus rules" of the QD scheme,

$$\begin{aligned} \hat{q}_k + \hat{e}_{k-1} &= q_k + e_k, \\ \hat{e}_{k-1}\hat{q}_{k-1} &= q_k e_{k-1}. \end{aligned}$$

For $\hat{q}_k$, $\hat{e}_k$ to be well defined, it must be assumed that $\hat{\pi}_n(z; z) \neq 0$ for all n, which by Lemma 1.56(a) is true, provided z is real and $\mathrm{d}\lambda$ positive definite.

1.7 Sobolev orthogonal polynomials

Classical orthogonal polynomials originated in connection with polynomial least squares problems. A relatively recent extension of the notion of orthogonality also was motivated by a least squares problem, namely to approximate a function simultaneously with some of its derivatives. This gives rise to an inner product involving derivatives,

$$(u, v)_S = (u, v)_{\mathrm{d}\lambda_0} + (u', v')_{\mathrm{d}\lambda_1} + \cdots + (u^{(s)}, v^{(s)})_{\mathrm{d}\lambda_s}, \tag{1.7.1}$$

where $\mathrm{d}\lambda_\sigma$ are positive measures not necessarily having the same support or being of the same type. Indeed, very often, $\mathrm{d}\lambda_0$ is absolutely continuous whereas some or all of the other measures $\mathrm{d}\lambda_\sigma$, $\sigma \geq 1$, are discrete. An inner product of the type (1.7.1) is called a *Sobolev inner product* (hence the subscript S on the left-hand inner product). *Positive definiteness* of $(\,\cdot\,,\,\cdot\,)_S$ is defined exactly as in Definition 1.1 for the case $s = 0$. In particular, $(\,\cdot\,,\,\cdot\,)_S$ is positive definite on $\mathbb{P}$ if $\mathrm{d}\lambda_0$ is, or if $\mathrm{d}\lambda_1$ is and $\int_{\mathbb{R}} \mathrm{d}\lambda_0(t) > 0$, etc.

The *Sobolev norm* is defined by

$$\|u\|_S = \sqrt{(u, u)_S} = \left(\sum_{\sigma=0}^{s} \int_{\mathbb{R}} [u^{(\sigma)}(t)]^2 \, \mathrm{d}\lambda_\sigma(t) \right)^{1/2}. \tag{1.7.2}$$

1.7.1 *Definition and properties*

Definition 1.58 *Monic real polynomials* $\pi_k(t) = t^k + \cdots$, $k = 0, 1, 2, \ldots$, *are called* monic orthogonal polynomials of Sobolev type *(or* Sobolev orthogonal polynomials *for short) with respect to the measures* $\mathrm{d}\lambda_\sigma$ *if*

$$\begin{gathered}(\pi_k, \pi_\ell)_S = 0 \quad \text{for } k \neq \ell, \quad k, \ell = 0, 1, 2, \ldots \text{ and} \\ \|\pi_k\|_S > 0 \quad \text{for } k = 0, 1, 2, \ldots \ .\end{gathered} \tag{1.7.3}$$

They will be denoted by $\pi_k(\,\cdot\,) = \pi_k(\,\cdot\,; S)$. *The* normalized *Sobolev orthogonal polynomials are* $\tilde{\pi}_k = \pi_k / \|\pi_k\|_S$, $k = 0, 1, 2, \ldots$.

Properties of the usual orthogonal polynomials which depend only on the basic properties of inner products and not on their particular form carry over immediately to Sobolev orthogonal polynomials. This is the case, in particular, for unique existence as well as extremal and symmetry properties. We simply state the respective facts.

Theorem 1.59 *If the inner product (1.7.1) is positive definite on* $\mathbb{P}$, *there exists a unique infinite sequence* $\{\pi_k(\,\cdot\,; S)\}$ *of monic orthogonal polynomials of Sobolev type.*

Theorem 1.60 *With* $\mathbb{P}_n^\circ$ *denoting the class of monic polynomials of degree* n, *there holds*

$$\|\pi\|_S \geq \|\pi_n(\,\cdot\,; S)\|_S \quad \text{for all } \pi \in \mathbb{P}_n^\circ,$$

with equality if and only if $\pi = \pi_n$.

Definition 1.61 *The Sobolev inner product (1.7.1) is called* symmetric *if each measure* $\mathrm{d}\lambda_\sigma$ *is symmetric in the sense of Definition 1.16.*

Theorem 1.62 *If the inner product (1.7.1) is symmetric, then*

$$\pi_k(-t; S) = (-1)^k \pi_k(t; S), \quad k = 0, 1, 2, \ldots \ .$$

1.7.2 *Recurrence relation and zeros*

The Sobolev inner product (1.7.1), when $s \geq 1$, no longer satisfies the shift property (1.3.1). In the case $s = 1$, for example, one finds

$$(tu, v)_S - (u, tv)_S = \int_{\mathbb{R}} (uv' - u'v)(t)\, \mathrm{d}\lambda_1(t),$$

which for $u(t) \equiv 1$, $v(t) = t$ gives $\int_{\mathbb{R}} \mathrm{d}\lambda_1(t) > 0$. As a consequence, one can no longer expect (cf. the proof of Theorem 1.27) to have three-term recurrence relations for Sobolev orthogonal polynomials. However, as for any sequence of monic polynomials whose degrees increase by 1 from one member to the next, they must satisfy a recurrence relation of the extended form

$$\pi_{k+1}(t) = t\pi_k(t) - \sum_{j=0}^{k} \beta_j^k \pi_{k-j}(t), \quad k = 0, 1, 2, \ldots \ . \tag{1.7.4}$$

Theorem 1.63 *The sequence of monic polynomials defined by (1.7.4) is orthogonal with respect to the Sobolev inner product (1.7.1) if and only if*

$$\beta_j^k = \frac{(t\pi_k, \pi_{k-j})_S}{(\pi_{k-j}, \pi_{k-j})_S}, \quad j = 0, 1, \ldots, k; \ k = 0, 1, 2, \ldots . \tag{1.7.5}$$

Proof (a) Assume $\pi_k(\,\cdot\,) = \pi_k(\,\cdot\,; S)$, $k = 0, 1, 2, \ldots$. Taking the inner product of both sides of (1.7.4) with π_{k-j} then gives

$$0 = (\pi_{k+1}, \pi_{k-j})_S = (t\pi_k, \pi_{k-j})_S - \beta_j^k (\pi_{k-j}, \pi_{k-j})_S, \quad j = 0, 1, \ldots, k,$$

from which (1.7.5) follows.

(b) Assume (1.7.5). Then $(\pi_1, \pi_0)_S = (t\pi_0, \pi_0)_S - \beta_0^0 (\pi_0, \pi_0)_S = 0$, that is, π_0 and π_1 are Sobolev-orthogonal. We proceed by induction on k. Suppose $\pi_0, \pi_1, \ldots, \pi_k$ is a system of monic Sobolev orthogonal polynomials. Then,

$$(\pi_{k+1}, \pi_{k-j})_S = (t\pi_k, \pi_{k-j})_S - \beta_j^k (\pi_{k-j}, \pi_{k-j})_S = 0, \quad j = 0, 1, \ldots, k.$$

Thus, the system $\pi_0, \pi_1, \ldots, \pi_k, \pi_{k+1}$ is also Sobolev-orthogonal. □

In cases of symmetry, the recurrence formula (1.7.4) simplifies.

Theorem 1.64 *If the inner product (1.7.1) is symmetric in the sense of Definition 1.61, then*

$$\beta_{2r}^k = 0, \quad r = 0, 1, \ldots, \lfloor k/2 \rfloor. \tag{1.7.6}$$

Proof In the inner product $(t\pi_k, \pi_{k-2r})_S$, the two members $t\pi_k$ and π_{k-2r} by Theorem 1.62 are polynomials of opposite parity, that is, one is even and the other odd, or vice versa, so that their product is odd. The same is true for all derivatives. By the symmetry of the measures $\mathrm{d}\lambda_\sigma$ it follows that $(t\pi_k, \pi_{k-2r})_S = 0$; hence, $\beta_{2r}^k = 0$. □

Let

$$\boldsymbol{H}_n = \begin{bmatrix} \beta_0^0 & \beta_1^1 & \beta_2^2 & \cdots & \beta_{n-2}^{n-2} & \beta_{n-1}^{n-1} \\ 1 & \beta_0^1 & \beta_1^2 & \cdots & \beta_{n-3}^{n-2} & \beta_{n-2}^{n-1} \\ 0 & 1 & \beta_0^2 & \cdots & \beta_{n-4}^{n-2} & \beta_{n-3}^{n-1} \\ \vdots & \vdots & \vdots & & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & \beta_0^{n-2} & \beta_1^{n-1} \\ 0 & 0 & 0 & \cdots & 1 & \beta_0^{n-1} \end{bmatrix} \tag{1.7.7}$$

be the $n \times n$ Hessenberg matrix of the coefficients β_j^k arranged upward in the kth column, and let

$$\boldsymbol{\pi}(t) = [\pi_0(t), \pi_1(t), \ldots, \pi_{n-1}(t)]^{\mathrm{T}}. \tag{1.7.8}$$

Theorem 1.65 *The zeros $\tau_1, \tau_2, \ldots, \tau_n$ of $\pi_n(\,\cdot\,; S)$ are the eigenvalues of $\boldsymbol{H}_n$, with $\boldsymbol{\pi}^{\mathrm{T}}(\tau_\nu)$ being a left eigenvector belonging to the eigenvalue τ_ν.*

Proof Write the first n equations of (1.7.4) in matrix form as

$$t\boldsymbol{\pi}^{\mathrm{T}}(t) = \boldsymbol{\pi}^{\mathrm{T}}(t)\boldsymbol{H}_n + \pi_n(t)\boldsymbol{e}_n^{\mathrm{T}},$$

where $\boldsymbol{e}_n^{\mathrm{T}} = [0, 0, \ldots, 1] \in \mathbb{R}^n$. Putting $t = \tau_\nu$ yields

$$\tau_\nu \boldsymbol{\pi}^{\mathrm{T}}(\tau_\nu) = \boldsymbol{\pi}^{\mathrm{T}}(\tau_\nu)\boldsymbol{H}_n, \quad \nu = 1, 2, \ldots, n,$$

which proves the assertion, since $\boldsymbol{\pi}^{\mathrm{T}}(\tau_\nu)$ is a nonzero vector, its first component being $\pi_0(\tau_\nu) = 1$. □

Remark In the case $s = 0$, one has $\beta_j^k = 0$ for $j > 0$, and the matrix $\boldsymbol{H}_n$ is tridiagonal. It can be symmetrized by a (real) diagonal similarity transformation and then becomes the Jacobi matrix $\boldsymbol{J}_n(\mathrm{d}\lambda_0)$ (cf. (1.3.15)). In the case $s > 0$, a symmetrization is no longer possible, since some of the eigenvalues of $\boldsymbol{H}_n$ may well be complex.

1.8 Orthogonal polynomials on the semicircle

In a sense, orthogonal polynomials on the semicircle are halfway between orthogonal polynomials on the real line and orthogonal polynomials on the unit circle. With the latter, they share the property of being complex-valued, with the former having the distinction of satisfying a three-term recurrence relation. We give a brief account of these polynomials, relegating some of the proofs to the literature.

1.8.1 *Definition, existence, and representation*

Let $w(z)$ be a weight function which is positive on $(-1, 1)$, has moments of all orders, and is extendible to a function analytic in the half-disk $D_+ = \{z \in \mathbb{C} : |z| < 1, \ \mathrm{Im}\, z > 0\}$. Let Γ be the circular part of ∂D_+. For the inner product (1.1.2) we now use the notation

$$[u, v] = \int_{-1}^{1} u(t)v(t)w(t)\,\mathrm{d}t, \tag{1.8.1}$$

and define, along with it, a complex inner product by

$$(u, v) = \int_\Gamma u(z)v(z)w(z)(\mathrm{i}z)^{-1}\,\mathrm{d}z = \int_0^\pi u(\mathrm{e}^{\mathrm{i}\theta})v(\mathrm{e}^{\mathrm{i}\theta})w(\mathrm{e}^{\mathrm{i}\theta})\,\mathrm{d}\theta, \tag{1.8.2}$$

assuming the integral exists for polynomials u and v. We further assume

$$\mathrm{Re}\,(1, 1) = \mathrm{Re} \int_0^\pi w(\mathrm{e}^{\mathrm{i}\theta})\,\mathrm{d}\theta \neq 0. \tag{1.8.3}$$

Note that the inner product (1.8.2) is not Hermitian, that is, $(u, u) = \|u\|^2$ is not necessarily real, let alone positive.

In slight deviation from the notation in Definition 1.3, the monic orthogonal polynomials with respect to the inner product (1.8.1) will be denoted by p_k,

$$[p_k, p_\ell] = 0 \quad \text{for } k \neq \ell, \quad p_k(t) = t^k + \cdots \,, \tag{1.8.4}$$

and the recurrence relation they satisfy by

$$y_{k+1} = (z - a_k)y_k - b_k y_{k-1}, \quad k = 0, 1, 2, \ldots \,. \tag{1.8.5}$$

Thus, if $y_{-1} = 0$, $y_0 = 1$, then $y_k = p_k(z)$; if $y_{-1} = -1$, $y_0 = 0$, then $y_k = q_k(z)$, where q_k are the polynomials of the second kind (denoted earlier by σ_k; cf. Theorem 1.39),

$$q_k(z) = \int_{-1}^{1} \frac{p_k(z) - p_k(t)}{z - t}\, w(t)\, \mathrm{d}t. \tag{1.8.6}$$

The moments associated with the inner products (1.8.1) and (1.8.2) will be denoted by m_r and μ_r, respectively,

$$m_r = [t^r, 1], \quad \mu_r = (t^r, 1), \quad r = 0, 1, 2, \ldots \,. \tag{1.8.7}$$

Recall that $b_0 = m_0$ and note that the quantity in (1.8.3) is $\operatorname{Re} \mu_0$.

The question of interest is whether or not the complex inner product (1.8.2) also admits a sequence of (complex) monic orthogonal polynomials π_k, and if so, how they are related to the polynomials p_k. The next theorem answers these questions in the affirmative.

Theorem 1.66 (Gautschi, Landau, and Milovanović, 1987) *Under assumption (1.8.3) and the assumptions made about the weight function w, there exists a unique system of (complex) monic orthogonal polynomials $\pi_k(\,\cdot\,) = \pi_k(\,\cdot\,; w)$ with respect to the inner product (1.8.2). In fact,*

$$\pi_n(z) = p_n(z) - \mathrm{i}\theta_{n-1} p_{n-1}(z), \quad n = 0, 1, 2, \ldots, \tag{1.8.8}$$

where

$$\theta_{n-1} = \frac{\mu_0 p_n(0) + \mathrm{i} q_n(0)}{\mathrm{i}\mu_0 p_{n-1}(0) - q_{n-1}(0)}\,, \quad n = 0, 1, 2, \ldots \,. \tag{1.8.9}$$

Alternatively,

$$\theta_n = \mathrm{i}a_n + \frac{b_n}{\theta_{n-1}}, \quad n = 0, 1, 2, \ldots; \quad \theta_{-1} = \mu_0, \tag{1.8.10}$$

where a_n, b_n are the recursion coefficients in (1.8.5) and $\mu_0 = (1, 1)$. In particular, if $a_n = 0$ for all n, then all θ_n are real (in fact, positive). Finally,

$$(\pi_n, \pi_n) = \theta_{n-1}[p_{n-1}, p_{n-1}] \neq 0, \quad n = 1, 2, 3, \ldots, \quad (\pi_0, \pi_0) = \mu_0. \tag{1.8.11}$$

Proof See Gautschi et al. (1987, pp. 392–393). □

The polynomials π_k of Theorem 1.66 are referred to as *orthogonal polynomials on the semicircle* relative to the weight function w. Equation (1.8.8) shows how they are related to the ordinary orthogonal polynomials p_k. The latter, conversely, can be expressed in terms of the former by (cf. Gautschi et al. (1987, eqn (2.17)))

$$p_n(z) = \sum_{k=0}^{n} \left(\prod_{\nu=k+1}^{n} \mathrm{i}\theta_{\nu-1} \right) \pi_k(z). \tag{1.8.12}$$

Example 1.67 $w(z) = (1-z)^\alpha (1+z)^\beta$, $\alpha > -1$, $\beta > -1$.

For real $z = x$ on $(-1, 1)$, this is the Jacobi weight function; see Table 1.1. For complex z, the fractional powers are to be understood in terms of their principal branches. The quantity μ_0 crucial for the existence of the polynomials π_k is $\mu_0 = \int_\Gamma w(z)(\mathrm{i}z)^{-1}\,\mathrm{d}z$. To compute it, we apply Cauchy's theorem, using the contour C_ε, $\varepsilon > 0$, consisting of ∂D_+ with a small semicircle of radius ε about the origin spared out. This gives

$$0 = \int_\Gamma w(z)(\mathrm{i}z)^{-1}\,\mathrm{d}z + \left(\int_{-1}^{-\varepsilon} + \int_{\varepsilon}^{1} \right) w(x)(\mathrm{i}x)^{-1}\,\mathrm{d}x + \int_{c_\varepsilon} w(z)(\mathrm{i}z)^{-1}\,\mathrm{d}z,$$

where c_ε is the upper semicircle of radius ε centered at the origin. Letting $\varepsilon \downarrow 0$, one gets

$$0 = \mu_0 - \mathrm{i} \int_{-1}^{1} \frac{w(x)}{x}\,\mathrm{d}x - \pi w(0),$$

where the integral is a Cauchy principal value integral, that is,

$$\mu_0 = \pi + \mathrm{i} \int_{-1}^{1} \frac{w(x)}{x}\,\mathrm{d}x.$$

Hence, $\operatorname{Re}\mu_0 \neq 0$, and the polynomials orthogonal on the semicircle with respect to the Jacobi weight function do indeed exist.

1.8.2 *Recurrence relation*

Since the inner product (1.8.2) clearly satisfies the shift property (1.3.1), the orthogonal polynomials π_k, if they exist, must satisfy a three-term recurrence relation. The precise details are contained in the following theorem.

Theorem 1.68 *Under assumption (1.8.3), the* (monic complex) *polynomials* $\pi_k(\,\cdot\,) = \pi_k(\,\cdot\,; w)$ *orthogonal with respect to the inner product (1.8.2) satisfy the recurrence relation*

$$\begin{aligned} \pi_{k+1}(z) &= (z - \mathrm{i}\alpha_k)\pi_k(z) - \beta_k \pi_{k-1}(z), \quad k = 0, 1, 2, \ldots, \\ \pi_{-1}(z) &= 0, \quad \pi_0(z) = 1, \end{aligned} \tag{1.8.13}$$

where the coefficients α_k, β_k *are given by*

$$\alpha_0 = \theta_0 - \mathrm{i}a_0, \quad \alpha_k = \theta_k - \theta_{k-1} - \mathrm{i}a_k, \quad k = 1, 2, 3, \ldots, \tag{1.8.14}$$

$$\beta_k = \theta_{k-1}(\theta_{k-1} - \mathrm{i}a_{k-1}), \quad k = 1, 2, 3, \ldots, \tag{1.8.15}$$

with θ_n defined in (1.8.9) [or (1.8.10)] *and a_n in (1.8.5).*

Remark to Theorem 1.68 The coefficient β_0 is arbitrary, but may conveniently be defined by $\beta_0 = \mu_0$. Alternative expressions for the α_k are

$$\alpha_0 = \frac{m_0}{\mu_0}, \quad \alpha_k = -\theta_{k-1} + \frac{b_k}{\theta_{k-1}}, \quad k = 1, 2, 3, \ldots,$$

where b_k are the coefficients in (1.8.5).

Proof Writing the three-term recurrence relation in the form (1.8.13), we determine α_k, β_k. Inserting (1.8.8) into (1.8.13) yields, for $k \geq 1$,

$$p_{k+1}(z) - \mathrm{i}\theta_k p_k(z) = (z - \mathrm{i}\alpha_k)[p_k(z) - \mathrm{i}\theta_{k-1}p_{k-1}(z)] - \beta_k[p_{k-1}(z) - \mathrm{i}\theta_{k-2}p_{k-2}(z)].$$

Now substitute $zp_k(z)$ and $zp_{k-1}(z)$ from the recurrence relation (1.8.5) to obtain

$$\begin{aligned}[a_k + \mathrm{i}(\theta_k - \theta_{k-1} - \alpha_k)]p_k(z) + [b_k - \beta_k - \theta_{k-1}(\alpha_k + \mathrm{i}a_{k-1})]p_{k-1}(z) \\ +\mathrm{i}[\beta_k\theta_{k-2} - b_{k-1}\theta_{k-1}]p_{k-2}(z) \equiv 0, \quad k \geq 1.\end{aligned}$$

Since $\{p_n\}$ are linearly independent, one concludes that

$$\begin{aligned} a_k + \mathrm{i}(\theta_k - \theta_{k-1} - \alpha_k) &= 0, \quad k \geq 1, \\ b_k - \beta_k - \theta_{k-1}(\alpha_k + \mathrm{i}a_{k-1}) &= 0, \quad k \geq 1, \\ \beta_k\theta_{k-2} - b_{k-1}\theta_{k-1} &= 0, \quad k \geq 2. \end{aligned} \tag{1.8.16}$$

The last relation in (1.8.16), in conjunction with (1.8.10), yields (1.8.15) for $k \geq 2$. The first relation in (1.8.16) gives (1.8.14) for $k \geq 1$. To verify (1.8.15) for $k = 1$, it suffices to apply the second relation in (1.8.16) for $k = 1$ and combine the result with (1.8.10) and (1.8.14) for $k = 1$. With α_k, β_k thus determined, the second relation in (1.8.16) is automatically satisfied, as one checks readily from (1.8.10). Finally, from $\pi_1(z) = z - \mathrm{i}\alpha_0 = p_1(z) - \mathrm{i}\theta_0 = z - a_0 - \mathrm{i}\theta_0$ one obtains the formula for α_0 in (1.8.14). □

The alternative formulae in the Remark follow from the relations (1.8.14) and (1.8.15) by applying (1.8.10).

The existence of the polynomials $\pi_k(\,\cdot\,; w)$ is guaranteed for any weight function w that is symmetric on $(-1, 1)$ and does not vanish at the origin.

Theorem 1.69 *If the weight function w satisfies*

$$w(-z) = w(z), \quad w(0) > 0, \tag{1.8.17}$$

then

$$\mu_0 = \pi w(0), \tag{1.8.18}$$

and the system of orthogonal polynomials $\{\pi_k(\,\cdot\,; w)\}$ exists uniquely.

Proof Proceeding as in Example 1.67, one finds

$$0 = \mu_0 - \mathrm{i} \fint_{-1}^{1} \frac{w(x)}{x} \mathrm{d}x - \pi w(0).$$

Here, the Cauchy principal value integral vanishes because of symmetry, and (1.8.18) follows. □

Symmetry also simplifies the formulae for the recursion coefficients in (1.8.13), since $a_k = 0$ for all $k \geq 0$. Hence,

$$\alpha_0 = \theta_0, \quad \alpha_k = \theta_k - \theta_{k-1}, \quad \beta_k = \theta_{k-1}^2 \quad (k \geq 1), \tag{1.8.19}$$

and by (1.8.10) and (1.8.18),

$$\left.\begin{aligned} \theta_0 &= \frac{m_0}{\pi w(0)}, \quad \theta_1 = \frac{b_1}{\theta_0}, \\ \theta_{2m} &= \theta_0 \, \frac{b_2 b_4 \cdots b_{2m}}{b_1 b_3 \cdots b_{2m-1}} \\ \theta_{2m+1} &= \frac{1}{\theta_0} \, \frac{b_1 b_3 \cdots b_{2m+1}}{b_2 b_4 \cdots b_{2m}} \end{aligned}\right\} \; m = 1, 2, 3, \ldots \; . \tag{1.8.20}$$

Example 1.70 Gegenbauer weight $w^{(\lambda)}(z) = (1 - z^2)^{\lambda - \frac{1}{2}}$, $\lambda > -\frac{1}{2}$.

Here (cf. Table 1.1)

$$\begin{aligned} m_0 &= \sqrt{\pi} \, \frac{\Gamma(\lambda + \frac{1}{2})}{\Gamma(\lambda + 1)}, \\ b_k &= \frac{k(k + 2\lambda - 1)}{4(k + \lambda)(k + \lambda - 1)}, \quad k = 1, 2, 3, \ldots, \end{aligned}$$

and from (1.8.20) one finds by induction

$$\theta_0 = \frac{1}{\sqrt{\pi}} \, \frac{\Gamma(\lambda + \frac{1}{2})}{\Gamma(\lambda + 1)}, \quad \theta_k = \frac{1}{\lambda + k} \, \frac{\Gamma(\frac{1}{2}(k+2))\Gamma(\lambda + \frac{1}{2}(k+1))}{\Gamma(\frac{1}{2}(k+1))\Gamma(\lambda + \frac{1}{2}k)}, \quad k \geq 1.$$

For $\lambda = \frac{1}{2}$ (i.e. $w(z) = 1$), this reduces to

$$\theta_k = \frac{2}{2k+1} \left(\frac{\Gamma(\frac{1}{2}(k+2))}{\Gamma(\frac{1}{2}(k+1))} \right)^2, \quad k \geq 0 \quad (w(z) = 1).$$

1.8.3 *Zeros*

Similarly as for ordinary and Sobolev orthogonal polynomials, the zeros of $\pi_n(\,\cdot\,) = \pi_n(\,\cdot\,; w)$, here too, can be characterized as eigenvalues of a certain matrix, this time a complex matrix, giving rise to complex eigenvalues.

We let again $\boldsymbol{\pi}(z) = [\pi_0(z), \pi_1(z), \ldots, \pi_{n-1}(z)]^{\mathrm{T}}$ and introduce the (complex tridiagonal) matrix

$$\boldsymbol{J}_n(w) = \begin{bmatrix} \mathrm{i}\alpha_0 & 1 & & & & 0 \\ \beta_1 & \mathrm{i}\alpha_1 & 1 & & & \\ & \beta_2 & \mathrm{i}\alpha_2 & 1 & & \\ & & \ddots & \ddots & \ddots & \\ & & & \beta_{n-2} & \mathrm{i}\alpha_{n-2} & 1 \\ 0 & & & & \beta_{n-1} & \mathrm{i}\alpha_{n-1} \end{bmatrix} \tag{1.8.21}$$

in order to write (1.8.13) in the form

$$z\boldsymbol{\pi}(z) = \boldsymbol{J}_n(w)\boldsymbol{\pi}(z) + \pi_n(z)\boldsymbol{e}_n. \tag{1.8.22}$$

In the same manner as before in §1.3.2 and §1.7.2, there follows:

Theorem 1.71 *The zeros $\tau_1, \tau_2, \ldots, \tau_n$ of $\pi_n(\,\cdot\,; w)$ are the eigenvalues of the matrix $\boldsymbol{J}_n(w)$ in (1.8.21), with $\boldsymbol{\pi}(\tau_\nu)$ being an eigenvector belonging to the eigenvalue τ_ν.*

If the weight function w is symmetric, then $\beta_k = \theta_{k-1}^2$ is positive (cf. (1.8.20)) and a similarity transformation with the diagonal matrix $\boldsymbol{D}_n = \mathrm{diag}(1, \mathrm{i}\theta_0, \mathrm{i}^2\theta_0\theta_1, \mathrm{i}^3\theta_0\theta_1\theta_2, \ldots) \in \mathbb{C}^{n\times n}$ transforms (1.8.21) into a real (nonsymmetric) tridiagonal matrix

$$-\mathrm{i}\boldsymbol{D}_n^{-1}\boldsymbol{J}_n(w)\boldsymbol{D}_n = \begin{bmatrix} \alpha_0 & \theta_0 & & & & 0 \\ -\theta_0 & \alpha_1 & \theta_1 & & & \\ & -\theta_1 & \alpha_2 & \theta_2 & & \\ & & \ddots & \ddots & \ddots & \\ & & & -\theta_{n-3} & \alpha_{n-2} & \theta_{n-2} \\ 0 & & & & -\theta_{n-2} & \alpha_{n-1} \end{bmatrix}. \tag{1.8.23}$$

The zeros τ_ν, therefore, are the eigenvalues of the real matrix on the right in (1.8.23) multiplied by i.

Example 1.72 Gegenbauer weight function $w^{(\lambda)}(z) = (1-z^2)^{\lambda-\frac{1}{2}}$, $\lambda > -\frac{1}{2}$.

It can be shown (Gautschi, Landau, and Milovanović, 1987, §6.3) that all zeros $\tau^{(\lambda)}$ of $\pi_n(\,\cdot\,; w^{(\lambda)})$, $n \geq 2$, are simple, distributed symmetrically with respect to the imaginary axis, and are all contained in the open half-disk $D_+ = \{z \in \mathbb{C} : |z| < 1, \mathrm{Im}\, z > 0\}$. The inclusion statement may well hold for arbitrary Jacobi weight functions $w^{(\alpha,\beta)}(z) = (1-z)^\alpha(1+z)^\beta$, but this is still a conjecture.

1.9 Notes to Chapter 1

The standard text on orthogonal polynomials is Szegö (1975). It deals largely with classical orthogonal polynomials and polynomials orthogonal on the unit circle. Many topics not considered in this book can be found there, among them asymptotics and inequalities of orthogonal polynomials and their zeros, and expansions in orthogonal polynomials. A text similar in outlook, though limited to polynomials on the real line, is Suetin (1979). The theory of orthogonal polynomials for more general measures of orthogonality is treated in Freud (1971) and, more recently, in Stahl and Totik (1992). The latter is a particularly rich source on nth-root asymptotics. Another useful source on asymptotics is Van Assche (1987), whereas Deift (1999) develops asymptotics from the rather different viewpoint of Riemann–Hilbert problems. A text strongly rooted in continued fraction theory and recurrence relations is Chihara (1978). For orthogonal polynomials with exponential weight functions, see the research monograph Levin and Lubinsky (2001). Orthogonal polynomials with respect to discrete measures are dealt with extensively in Nikiforov, Suslov, and Uvarov (1991). The roles of classical orthogonal polynomials in algebraic combinatorics, or in stochastic processes, are discussed, respectively, in Bannai (1990) and Schoutens (2000). Bultheel and Van Barel (1997) consider orthogonal polynomials in the context of rational approximation and linear algebra.

While in this book only polynomials are considered that are orthogonal relative to a single measure, there are interesting polynomials—the so-called *multiple orthogonal polynomials*—that satisfy orthogonality relations relative to a finite number r of measures supported either on mutually distinct intervals, or on one common interval. These arise in simultaneous rational approximation of r functions. For a detailed account of multiple orthogonal polynomials, see Aptekarev (1998) and Nikishin and Sorokin (1991, Chapter 4), for a number of concrete examples involving continuous and discrete measures Van Assche and Coussement (2001), Coussement and Van Assche (2003), Aptekarev, Branquinho, and Van Assche (2003), Arvesú, Coussement, and Van Assche (2003), Beckermann, Coussement, and Van Assche (2004), and for computational aspects Milovanović and Stanić (2003).

For recent expositions of orthogonal polynomials on the unit circle and related quadrature methods, see, for example, Jones, Njåstad, and Thron (1989), Gragg (1993), Bultheel, González-Vera, Hendriksen, and Njåstad (1994), Daruis and González-Vera (2001), and Bultheel, Daruis, and González-Vera (2001), the last work exhibiting the close connection between Gauss quadrature formulae on $[-1, 1]$ and Szegö quadrature formulae on the unit circle for measures appropriately related. For Jacobi-type weight functions, Szegö orthogonal polynomials and quadrature rules have been obtained in Daruis, González-Vera, and Njåstad (2001). Rational Szegö quadrature formulae exact on spaces of rational functions having prescribed poles are discussed in Bultheel, González-Vera, Hendriksen, and Njåstad (2001). Formally orthogonal polynomials on arcs in the complex plane and related (complex) Gaussian quadrature formulae are consid-

ered in Saylor and Smolarski (2001) in connection with the biconjugate gradient algorithm of numerical linear algebra.

Orthogonal polynomials of several variables and matrix orthogonal polynomials are beyond the scope of this book. For the former, see, for example, Dunkl and Xu (2001), and for the latter, Sinap and Van Assche (1996) and Freund (2001).

§1.1. There is a theory of *formal orthogonal polynomials* which is based on three-term recurrence relations with arbitrary real or complex coefficients α_k, $\beta_k \neq 0$, and associated complex Jacobi matrices (cf. also §1.6). These are of considerable interest in such areas as the iterative solution of large systems of linear algebraic equations and Padé approximation. For a recent account, see Beckermann (2001).

§1.2.4. There is some work, particularly by Italian researchers, on s-orthogonal polynomials and generalizations thereof, called σ-orthogonal polynomials; see, for example, Gautschi (1981b, §2.2.3). Interestingly, the Chebyshev polynomials T_n (cf. Table 1.1) are s-orthogonal on $[-1, 1]$ for each $s = 0, 1, 2, \ldots$ with respect to the Chebyshev weight function $w(t) = (1 - t^2)^{-1/2}$.

§1.3. For Jacobi matrices that are positive definite (and hence have only positive eigenvalues), one can use the Cholesky decomposition of the Jacobi matrix to arrive at a pair of coupled two-term recurrence relations. The potential advantages of two-term vs three-term recursion are discussed in Laurie (1999b).

§1.4.1. It is difficult to trace the origin of Theorem 1.45. Jacobi must have been aware of it; the technique in the proof of this theorem of dividing one polynomial by another is due to Jacobi (1826).

§1.4.2. Gauss (1814), in an attempt to improve upon the Newton–Cotes formula, discovered the quadrature rule named after him in the simplest case $\mathrm{d}\lambda(t) = \mathrm{d}t$ on $[-1, 1]$ using continued fractions. The generalization to arbitrary weight functions is due to Christoffel (1877). The original reference to Theorem 1.48 is Markoff (1885).

Gauss-type quadrature rules (with $\mathrm{d}\lambda(t) = \mathrm{d}t$) having prescribed nodes on the boundary of, or outside, the support interval have been studied already by Christoffel (1858). Radau's formula, which is a special case, is mentioned in Radau (1880), while the Lobatto formula appears in Lobatto (1852). Anti-Gauss rules, introduced by Laurie (1996), are $(n + 1)$-point rules having degree of exactness $2n - 1$, which integrate polynomials of degree $2n + 1$ with an error that is equal in modulus, but opposite in sign, to the error of the n-point Gauss rule. Modified anti-Gauss rules are defined and applied to two-sided estimation of integrals in Calvetti and Reichel (2003a).

The problem of approximating r (> 1) weighted integrals of the same function by a Gauss-like quadrature rule having the same set of nodes has been considered in Borges (1994). Although not explicitly stated by the author, the problem is related to multiple orthogonal polynomials.

Extensions of Gaussian quadrature formulae to matrix-valued weight functions and their relation to orthogonal matrix polynomials is discussed in Durán

and Polo (2002) and Durán and Defez (2002). Other generalizations involve exactness for systems of nonpolynomial functions. For recent work on this, including computational algorithms, see Cheng, Rokhlin, and Yarvin (1999); the case of rational functions is discussed in §3.1.4.

§1.6. Kernel polynomials for positive definite measures $\mathrm{d}\lambda$ were introduced by Stiefel (1958) and applied to problems of numerical linear algebra. For the extension to quasi-definite measures, see Chihara (1978). The exposition in §1.6 follows closely the treatment in Gautschi (1982a). The argumentation in the proof of Theorem 1.57 goes back to Stiefel (1958, §5), but does not require the assumption of positive definiteness of $(\,\cdot\,,\,\cdot\,)_{\mathrm{d}\lambda}$. The second remark to Theorem 1.57 is due to Chinellato (2003).

§1.7. Simultaneous least squares approximation to a function and its derivatives has already been studied by Lewis (1947), where the emphasis is on the Peano representation of the error. The use, in this context, of polynomials orthogonal with respect to a Sobolev inner product was first suggested by Althammer (1962), who considered $s = 1$, $\mathrm{d}\lambda_0(t) = \mathrm{d}t$, $\mathrm{d}\lambda_1(t) = \gamma\,\mathrm{d}t$ on $[-1, 1]$ where $\gamma > 0$ is a constant. The problem, and in particular the polynomials involved, were subsequently studied by Gröbner (1967) and Brenner (1969). Since these early days, the literature on the subject has mushroomed enormously, most of the work having been done for its own sake, with little regard to applications. Recent surveys can be found in Marcellán, Alfaro, and Rezola (1993), Marcellán, Pérez, Piñar, and Ronveaux (1996), Meijer (1996), and an extensive bibliography in Marcellán and Ronveaux (1995).

For very special measures there are recurrence relations of a different type, which are shorter than (1.7.4); see, for example, Marcellán and Ronveaux (1990), Evans, Littlejohn, Marcellán, Markett, and Ronveaux (1995), Gautschi (1997c), and the Notes to §2.5.

§1.8. Polynomials orthogonal on the semicircle were first introduced by Gautschi and Milovanović (1986a) and given a more definitive treatment in Gautschi, Landau, and Milovanović (1987). The theory has been extended to arbitrary arcs in the complex plane by de Bruin (1990), Milovanović and Rajković (1990), (1994). For polynomials orthogonal on radial rays in the complex plane, see Milovanović (2002), and Milovanović and Cvetković (2004) for polynomials formally orthogonal with respect to the complex measure $\mathrm{d}\lambda(t) = t\mathrm{e}^{\mathrm{i}mt}\,\mathrm{d}t$ on $[-1, 1]$.

2

COMPUTATIONAL METHODS

The fundamental problem is to compute the first n recursion coefficients $\alpha_k(\mathrm{d}\lambda)$, $\beta_k(\mathrm{d}\lambda)$, $k = 0, 1, \ldots, n-1$ (cf. §1.3.1), where $n \geq 1$ is a (typically large) integer and $\mathrm{d}\lambda$ a positive measure given either implicitly via moment information or explicitly. In the former case, an important aspect is the sensitivity of the problem with respect to small perturbations in the data (the first $2n$ moments or modified moments); this is the question of conditioning. In principle, there is a simple algorithm, essentially due to Chebyshev, that produces the desired recursion coefficients from given moment information. The effectiveness of this algorithm, however, depends critically on the conditioning of the underlying problem. If the problem is ill-conditioned, as it often is, recourse has to be made either to symbolic computation or to the explicit form of the measure. A procedure applicable in the latter case is discretization of the measure and subsequent approximation of the desired recursion coefficients by those relative to a discrete measure.

Other problems calling for numerical methods are the evaluation of Cauchy integrals of orthogonal polynomials and the problem of passing from the recursion coefficients of a measure to those of a modified measure—the original measure multiplied by a rational function. Finally, Sobolev orthogonal polynomials present their own problems of calculating recursion coefficients and zeros.

2.1 Moment-based methods

Orthogonal polynomials as well as their recursion coefficients are expressible in determinantal form in terms of the moments of the underlying measure. Indeed, much of the classical theory of orthogonal polynomials is moment-oriented. This is true, in particular, of a classical algorithm due to Chebyshev, which generates the recursion coefficients directly from the moments, bypassing determinants.

The use of moments, unfortunately, is numerically problematic inasmuch as they give rise to severe ill-conditioning. In many cases, particularly for measures with bounded support, it is possible, however, to work with the so-called "modified moments," which lead to better conditioned problems and a more stable analog of the Chebyshev algorithm.

2.1.1 *Classical approach via moment determinants*

As in (1.1.5), we let Δ_n denote the Hankel determinant of order n in the moments $\mu_r = \mu_r(\mathrm{d}\lambda)$ given by (1.1.1),

$$\Delta_0 = 1, \quad \Delta_n = \begin{vmatrix} \mu_0 & \mu_1 & \cdots & \mu_{n-1} \\ \mu_1 & \mu_2 & \cdots & \mu_n \\ \vdots & \vdots & & \vdots \\ \mu_{n-1} & \mu_n & \cdots & \mu_{2n-2} \end{vmatrix}, \quad n = 1, 2, 3, \dots . \tag{2.1.1}$$

In addition, we define

$$\Delta_0' = 0, \quad \Delta_1' = \mu_1, \quad \Delta_n' = \begin{vmatrix} \mu_0 & \mu_1 & \cdots & \mu_{n-2} & \mu_n \\ \mu_1 & \mu_2 & \cdots & \mu_{n-1} & \mu_{n+1} \\ \vdots & \vdots & & \vdots & \vdots \\ \mu_{n-1} & \mu_n & \cdots & \mu_{2n-3} & \mu_{2n-1} \end{vmatrix}, \quad n = 2, 3, \dots . \tag{2.1.2}$$

Thus, Δ_n' is the Hankel determinant Δ_{n+1} with the penultimate column and the last row removed. By transposition, this is the same as the Hankel determinant Δ_{n+1} with the penultimate row and the last column removed.

Theorem 2.1 *Let $\pi_k(\,\cdot\,) = \pi_k(\,\cdot\,; \mathrm{d}\lambda)$ be the monic orthogonal polynomial of degree k with respect to the measure* $\mathrm{d}\lambda$ (cf. Definition 1.3). *Then,*

$$\pi_k(t) = \frac{1}{\Delta_k} \begin{vmatrix} \mu_0 & \mu_1 & \cdots & \mu_k \\ \mu_1 & \mu_2 & \cdots & \mu_{k+1} \\ \vdots & \vdots & & \vdots \\ \mu_{k-1} & \mu_k & \cdots & \mu_{2k-1} \\ 1 & t & \cdots & t^k \end{vmatrix} = t^k - \frac{\Delta_k'}{\Delta_k} t^{k-1} + \cdots, \quad k = 1, 2, \dots . \tag{2.1.3}$$

Proof The determinantal expression in (2.1.3) is clearly a monic polynomial of degree k. Denote it by $d_k(t)$. Let $C_0, C_1, \dots, C_k$ be the (signed) cofactors of the elements in the last row of Δ_{k+1}. From

$$t^r d_k(t) = \frac{1}{\Delta_k} \begin{vmatrix} \mu_0 & \mu_1 & \cdots & \mu_k \\ \mu_1 & \mu_2 & \cdots & \mu_{k+1} \\ \vdots & \vdots & & \vdots \\ \mu_{k-1} & \mu_k & \cdots & \mu_{2k-1} \\ t^r & t^{r+1} & \dots & t^{r+k} \end{vmatrix},$$

using Laplace expansion of the determinant with respect to the last row, one gets

$$t^r d_k(t) = \frac{1}{\Delta_k} \sum_{\ell=0}^{k} C_\ell t^{r+\ell}.$$

Thus, upon integration,

$$\int_{\mathbb{R}} t^r d_k(t)\, \mathrm{d}\lambda(t) = \frac{1}{\Delta_k} \sum_{\ell=0}^{k} C_\ell \mu_{r+\ell} = 0, \quad r = 0, 1, \dots, k-1,$$

since the sum is the Laplace expansion with repect to the last row of the Hankel determinant Δ_{k+1} in which the last row has been replaced by one of the earlier

rows. This proves orthogonality of d_k to all polynomials of lower degree; hence, by uniqueness, $d_k \equiv \pi_k$. The coefficient of t^{k-1} in the determinant of (2.1.3) is the (signed) cofactor of t^{k-1}, which is $-\Delta_k'$. □

Theorem 2.2 *The recursion coefficients* $\alpha_k = \alpha_k(\mathrm{d}\lambda)$, $\beta_k = \beta_k(\mathrm{d}\lambda)$ (cf. Theorem 1.27) *for the monic orthogonal polynomials* $\pi_k(\,\cdot\,;\mathrm{d}\lambda)$ *are given by*

$$\alpha_k = \frac{\Delta_{k+1}'}{\Delta_{k+1}} - \frac{\Delta_k'}{\Delta_k}, \quad k = 0, 1, 2, \ldots, \tag{2.1.4}$$

$$\beta_k = \frac{\Delta_{k+1}\Delta_{k-1}}{\Delta_k^2}, \quad k = 1, 2, 3, \ldots\ . \tag{2.1.5}$$

Proof By (1.3.3) and (1.3.4), one has

$$\alpha_k = \frac{(t\pi_k, \pi_k)}{(\pi_k, \pi_k)}, \quad k \geq 0; \quad \beta_k = \frac{(\pi_k, \pi_k)}{(\pi_{k-1}, \pi_{k-1})}, \quad k \geq 1.$$

On the other hand, using (2.1.3),

$$(t\pi_k, \pi_k) = \left(t^{k+1} - \frac{\Delta_k'}{\Delta_k}\, t^k + \cdots, \pi_k\right) = (t^{k+1}, \pi_k) - \frac{\Delta_k'}{\Delta_k}\,(t^k, \pi_k),$$

which holds also for $k = 0$. By an argument similar to the one in the proof of Theorem 2.1 and noting the sentence immediately preceding Theorem 2.1, one finds

$$(t^{k+1}, \pi_k) = \frac{\Delta_{k+1}'}{\Delta_k}, \quad (t^k, \pi_k) = (\pi_k, \pi_k) = \frac{\Delta_{k+1}}{\Delta_k}.$$

Therefore,

$$\alpha_k = \left(\frac{\Delta_{k+1}'}{\Delta_k} - \frac{\Delta_k'}{\Delta_k}\,\frac{\Delta_{k+1}}{\Delta_k}\right) \Big/ \frac{\Delta_{k+1}}{\Delta_k} = \frac{\Delta_{k+1}'}{\Delta_{k+1}} - \frac{\Delta_k'}{\Delta_k},$$

$$\beta_k = \frac{\Delta_{k+1}}{\Delta_k} \Big/ \frac{\Delta_k}{\Delta_{k-1}} = \frac{\Delta_{k+1}\Delta_{k-1}}{\Delta_k^2}.$$

□

Remark to Theorem 2.2 If one defines $\Delta_{-1} = 1$, eqn (2.1.5) holds also for $k = 0$, since $\Delta_1 = \mu_0 = \beta_0$ (cf. (1.3.6)).

The formulae (2.1.4) and (2.1.5) are not recommended as a method for computing the recursion coefficients. For one, they require the evaluation of determinants or, equivalently, triangular factorization of the respective matrices. This can be bypassed by Chebyshev's algorithm (cf. §2.1.7). For another, the problem solved by (2.1.4) and (2.1.5), namely the computation of the coefficients $\alpha_k(\mathrm{d}\lambda)$ and $\beta_k(\mathrm{d}\lambda)$, from the moments of $\mathrm{d}\lambda$, can be severely ill-conditioned (cf. §2.1.6). Nevertheless, formulae (2.1.4) and (2.1.5), when evaluated in higher-precision arithmetic, do have applications, for example, in testing the accuracy of the nodes and weights of Gaussian quadrature rules; cf. Gautschi (1983).

2.1.2 *Condition of nonlinear maps*

Consider first the simplest map $\mathbb{R} \to \mathbb{R}$ defined by $y = f(x)$, where f is a real-valued nonlinear function of a real variable x. With x assumed fixed, our interest is in the effect of a small perturbation Δx of x upon the value y of f. We denote by Δy the change in y caused by Δx. Assuming f differentiable at x, one has by Taylor's formula

$$\Delta y \approx f'(x)\Delta x, \tag{2.1.6}$$

an approximation that, in the limit as $\Delta x \to 0$, becomes an identity. Thus, in terms of *absolute* perturbations, the value of $|f'(x)|$ measures the sensitivity of f at the point x with respect to small perturbations.

Definition 2.3 *If $f : \mathbb{R} \to \mathbb{R}$ is differentiable at the point x, then*

$$(\mathrm{cond}_{\mathrm{abs}}\, f)(x) = |f'(x)| \tag{2.1.7}$$

is called the absolute condition number *of f at the point x.*

In practice, it is often more relevant to know the sensitivity of f in terms of *relative* perturbations. Thus, assuming $x \neq 0$ and $y = f(x) \neq 0$, writing (2.1.6) equivalently as

$$\frac{\Delta y}{y} \approx \frac{x f'(x)}{f(x)} \frac{\Delta x}{x} \tag{2.1.8}$$

motivates the following definition.

Definition 2.4 *If $f : \mathbb{R} \to \mathbb{R}$ is differentiable at $x \neq 0$ and $y = f(x) \neq 0$, then*

$$(\mathrm{cond}_{\mathrm{rel}}\, f)(x) = \left| \frac{x f'(x)}{f(x)} \right| \tag{2.1.9}$$

is called the relative condition number *of f at x.*

Remark to Definition 2.4 If $x = 0$ and $y \neq 0$, one should consider an absolute perturbation of x and a relative perturbation of y, and the other way around if $x \neq 0$ and $y = f(x) = 0$. The respective condition numbers then are $(\mathrm{cond}\, f)(x) = |f'(x)/f(x)|$ and $(\mathrm{cond}\, f)(x) = |x f'(x)|$. If $x = y = 0$, the appropriate condition number is the one in Definition 2.3. Since these modifications create discontinuities in the behavior of the condition number, it is preferable, and in fact quite natural, to use relative error only if the quantity in question is greater than 1 in modulus, and absolute error otherwise. This gives rise to the *mollified condition number*

$$(\mathrm{cond}_{\mathrm{mol}}\, f)(x) = \frac{m(x)|f'(x)|}{m(f(x))}\,, \tag{2.1.10}$$

where $m(\,\cdot\,)$ is the *mollifier function*

$$m(t) = \begin{cases} 1 & \text{if } |t| < 1, \\ |t| & \text{otherwise.} \end{cases} \tag{2.1.11}$$

A map $f : \mathbb{R} \to \mathbb{R}$ is called *ill-conditioned* at the point x if its condition number at x is much larger than 1 (typically by many decimal orders of magnitude) and *well-conditioned* otherwise. A condition number of the order 10^d means roughly a loss of d decimal digits when the data are perturbed by one unit in the last decimal. Whether or not this is acceptable depends both on the accuracy desired and the precision available. For example, if the working precision is 15 decimal digits, and the condition number is 10^8, the result will be accurate to about $15 - 8 = 7$ digits, which is acceptable if one needs 7-digit accuracy or less.

Suppose now that $\boldsymbol{f}$ is a map $\mathbb{R}^m \to \mathbb{R}^n$ defined by $\boldsymbol{y} = \boldsymbol{f}(\boldsymbol{x})$, where $\boldsymbol{f} = [f_1, f_2, \ldots, f_n]^{\mathrm{T}}$ is a vector of n nonlinear real-valued functions $f_\nu = f_\nu(\boldsymbol{x})$ in m real variables $\boldsymbol{x} = [x_1, x_2, \ldots, x_m]^{\mathrm{T}}$. The analog of the derivative in (2.1.6) then is the *Fréchet derivative*

$$\frac{\partial \boldsymbol{f}(\boldsymbol{x})}{\partial \boldsymbol{x}} = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & \cdots & \frac{\partial f_1}{\partial x_m} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} & \cdots & \frac{\partial f_2}{\partial x_m} \\ \vdots & \vdots & & \vdots \\ \frac{\partial f_n}{\partial x_1} & \frac{\partial f_n}{\partial x_2} & \cdots & \frac{\partial f_n}{\partial x_m} \end{bmatrix} (\boldsymbol{x}), \tag{2.1.12}$$

that is, the linear transformation defined by the Jacobian matrix of $\boldsymbol{f}$ at $\boldsymbol{x}$. This suggests

Definition 2.5 *If $\boldsymbol{f} : \mathbb{R}^m \to \mathbb{R}^n$ is Fréchet-differentiable at the point $\boldsymbol{x} \in \mathbb{R}^m$, then*

$$(\mathrm{cond}_{\mathrm{abs}}\, \boldsymbol{f})(\boldsymbol{x}) = \left\| \frac{\partial \boldsymbol{f}(\boldsymbol{x})}{\partial \boldsymbol{x}} \right\|, \tag{2.1.13}$$

where the norm on the right is an appropriate matrix norm, is called the absolute condition number *of $\boldsymbol{f}$ at $\boldsymbol{x}$.*

Since orders of magnitude is all that counts when considering the conditioning of maps, and since matrix norms are equivalent, the choice of norm in (2.1.13) is not all that critical. Choices frequently made are either the *infinity norm*

$$\left\| \frac{\partial \boldsymbol{f}(\boldsymbol{x})}{\partial \boldsymbol{x}} \right\|_\infty = \max_{1 \le \nu \le n} \sum_{\mu=1}^{m} \left| \frac{\partial f_\nu(\boldsymbol{x})}{\partial x_\mu} \right|, \tag{2.1.14}$$

or the *Frobenius norm*

$$\left\| \frac{\partial \boldsymbol{f}(\boldsymbol{x})}{\partial \boldsymbol{x}} \right\|_F = \left(\sum_{\mu=1}^{m} \sum_{\nu=1}^{n} \left| \frac{\partial f_\nu(\boldsymbol{x})}{\partial x_\mu} \right|^2 \right)^{1/2}. \tag{2.1.15}$$

In analogy to Definition 2.4, one can define a relative condition number as follows.

Definition 2.6 *Let* $\boldsymbol{f}: \mathbb{R}^m \to \mathbb{R}^n$ *be Fréchet-differentiable at* $\boldsymbol{x} = [x_1, x_2, \ldots, x_m]^{\mathrm{T}}$, *where* $x_\mu \neq 0$, $\mu = 1, 2, \ldots, m$, *and* $\boldsymbol{y} = \boldsymbol{f}(\boldsymbol{x}) = [y_1, y_2, \ldots, y_n]^{\mathrm{T}}$ *be such that* $y_\nu = f_\nu(\boldsymbol{x}) \neq 0$, $\nu = 1, 2, \ldots, n$. *Let* $\boldsymbol{C}(\boldsymbol{x}) \in \mathbb{R}^{n\times m}$ *be defined by*

$$\boldsymbol{C}(\boldsymbol{x}) = [c_{\nu\mu}(\boldsymbol{x})], \quad c_{\nu\mu}(\boldsymbol{x}) = \left| \frac{x_\mu(\partial f_\nu(\boldsymbol{x})/\partial x_\mu)}{f_\nu(\boldsymbol{x})} \right|, \quad \nu = 1, \ldots, n;\ \mu = 1, \ldots, m. \tag{2.1.16}$$

Then, a relative condition number *of* $\boldsymbol{f}$ *at* $\boldsymbol{x}$ *may be defined by*

$$(\mathrm{cond}_{\mathrm{rel}}\, \boldsymbol{f})(\boldsymbol{x}) = \|\boldsymbol{C}(\boldsymbol{x})\|, \tag{2.1.17}$$

where the norm on the right is an appropriate matrix norm. If one of the components of $\boldsymbol{x}$ *or of* $\boldsymbol{f}(\boldsymbol{x})$ *vanishes,* $c_{\nu\mu}(\boldsymbol{x})$ *must be modified as described in Remark to Definition 2.4. Using the mollifier function (2.1.11), one may also take*

$$c_{\nu\mu}(\boldsymbol{x}) = \frac{m(x_\mu)|\partial f_\nu(\boldsymbol{x})/\partial x_\mu|}{m(f_\nu(\boldsymbol{x}))}\,. \tag{2.1.18}$$

Definition 2.6 provides the most detailed description of the conditioning of $\boldsymbol{f}$ in terms of relative perturbations. It essentially takes each component f_ν of $\boldsymbol{f}$ and measures its relative condition with respect to one single variable x_μ; this is the meaning of $c_{\nu\mu}(\boldsymbol{x})$. One can thus think of $\boldsymbol{C}(\boldsymbol{x})$ as a relative *condition matrix*. To obtain a *condition number*, one takes a norm of $\boldsymbol{C}(\boldsymbol{x})$.

Remark to Definition 2.6 A simpler, but less detailed, definition of a relative condition number, which is meaningful for any $\boldsymbol{x} \neq \boldsymbol{0}$ and $\boldsymbol{f} \neq \boldsymbol{0}$, is

$$(\mathrm{cond}_{\mathrm{rel}}\, \boldsymbol{f})(\boldsymbol{x}) = \frac{\|\boldsymbol{x}\|_{\mathbb{R}^m}\, \|\partial \boldsymbol{f}(\boldsymbol{x})/\partial \boldsymbol{x}\|_{\mathbb{R}^{n\times m}}}{\|\boldsymbol{f}(\boldsymbol{x})\|_{\mathbb{R}^n}}\,, \tag{2.1.19}$$

where the norms on the right are suitable vector and matrix norms. In general, however, the condition number so defined can be misleading, since norms have a tendency to destroy detail. A simple instance of this is given in Gautschi (1997b, Chapter 1, p. 26) and more relevant instances are discussed in Examples 2.15 and 2.16.

2.1.3 *The moment maps* $\boldsymbol{G}_n$ *and* $\boldsymbol{K}_n$

There are several moment maps of interest in computing orthogonal polynomials, depending on what is to be computed and from what kind of moment information. A first map, denoted by $\boldsymbol{G}_n$, relates to the computation of n-point Gauss quadrature rules, that is, the computation of the n weights $\lambda_\nu = \lambda_\nu^G$ and n nodes $\tau_\nu = \tau_\nu^G$ in (1.4.7). These are collected in the vector

$$\boldsymbol{\gamma} = \boldsymbol{\gamma}(\mathrm{d}\lambda) = [\lambda_1, \lambda_2, \ldots, \lambda_n, \tau_1, \tau_2, \ldots, \tau_n]^{\mathrm{T}}. \tag{2.1.20}$$

The simplest, but what turns out to be an ill-conditioned, map $\boldsymbol{G}_n$ is the one that takes the first $2n$ moments

$$\boldsymbol{\mu} = \boldsymbol{\mu}(\mathrm{d}\lambda) = [\mu_0, \mu_1, \ldots, \mu_{2n-1}]^{\mathrm{T}}, \quad \mu_r = \int_{\mathbb{R}} t^r \, \mathrm{d}\lambda(t), \tag{2.1.21}$$

into the vector $\boldsymbol{\gamma}$,

$$\boldsymbol{G}_n : \ \mathbb{R}^{2n} \to \mathbb{R}^{2n} \quad \boldsymbol{\mu} \mapsto \boldsymbol{\gamma}. \tag{2.1.22}$$

Other, hopefully better conditioned, maps $\boldsymbol{G}_n$ take as input *modified moments* $\boldsymbol{m} = \boldsymbol{m}(\mathrm{d}\lambda) = [m_0, m_1, \ldots, m_{2n-1}]^{\mathrm{T}}$. In the most general case, these are defined in terms of a basis $\{p_k\}_{k=0}^{2n-1}$ of $\mathbb{P}_{2n-1}$, where $p_k = p_{k,n}$ may depend on n. In fact,

$$m_k = m_k(\mathrm{d}\lambda) := \int_{\mathbb{R}} p_k(t) \, \mathrm{d}\lambda(t), \quad k = 0, 1, \ldots, 2n-1, \tag{2.1.23}$$

and

$$\boldsymbol{G}_n : \ \mathbb{R}^{2n} \to \mathbb{R}^{2n} \quad \boldsymbol{m} \mapsto \boldsymbol{\gamma}. \tag{2.1.24}$$

Example 2.7 *Powers* $p_k(t) = t^k$, $k = 0, 1, \ldots, 2n-1$. In this case, $\boldsymbol{m} = \boldsymbol{\mu}$ and one has the map $\boldsymbol{G}_n$ of (2.1.22).

Example 2.8 *Orthogonal polynomials* $p_k(\,\cdot\,) = p_k(\,\cdot\,; \mathrm{d}\ell)$, $k = 0, 1, \ldots, 2n-1$, the first $2n$ monic polynomials orthogonal with respect to a positive measure $\mathrm{d}\ell$. (Nonmonic orthogonal polynomials are also used sometimes.) By choosing $\mathrm{d}\ell$ near $\mathrm{d}\lambda$ in some sense, one hopes to arrive at a map $\boldsymbol{G}_n$ in (2.1.24) that is well, or at least better, conditioned (cf., e.g. Example 2.29).

Example 2.9 *Bernstein polynomials* $p_{k,n}(t) = B_{k,n}(t)$, $t \in [0, 1]$, where

$$B_{k,n}(t) = \binom{2n-1}{k} t^k (1-t)^{2n-1-k}, \quad k = 0, 1, \ldots, 2n-1. \tag{2.1.25}$$

These are appropriate for measures $\mathrm{d}\lambda$ supported on $[0, 1]$.

Example 2.10 *Lagrange interpolation polynomials.* Given $2n$ distinct nodes $t_0, t_1, \ldots, t_{2n-1}$ in the support interval of $\mathrm{d}\lambda$, one takes

$$p_{k,n}(t) = \ell_{k,2n}(t), \quad \ell_{k,2n}(t) = \prod_{\substack{\ell=0 \\ \ell \neq k}}^{2n-1} \frac{t - t_\ell}{t_k - t_\ell}, \quad k = 0, 1, \ldots, 2n-1. \tag{2.1.26}$$

The second type of map, $\boldsymbol{K}_n$, relates to the computation of the first $2n$ recursion coefficients $\alpha_\nu = \alpha_\nu(\mathrm{d}\lambda)$, $\beta_\nu = \beta_\nu(\mathrm{d}\lambda)$, $\nu = 0, 1, 2, \ldots, n-1$ (cf. §1.3.1), which again are collected in a vector

$$\boldsymbol{\rho} = \boldsymbol{\rho}(\mathrm{d}\lambda) = [\alpha_0, \ldots, \alpha_{n-1}, \beta_0, \ldots, \beta_{n-1}]^{\mathrm{T}}. \tag{2.1.27}$$

Thus,

$$\boldsymbol{K}_n : \ \mathbb{R}^{2n} \to \mathbb{R}^{2n} \quad \boldsymbol{\mu} \ (\text{resp. } \boldsymbol{m}) \ \mapsto \boldsymbol{\rho}, \tag{2.1.28}$$

where, as before, $\boldsymbol{\mu}$ resp. $\boldsymbol{m}$ is the vector of the first $2n$ ordinary resp. modified moments. The latter are defined in (2.1.23) and may be chosen as in Examples 2.7–2.10.

In principle, the map $\boldsymbol{K}_n$ can be represented as a composition of two maps,

$$\boldsymbol{K}_n = \boldsymbol{H}_n \circ \boldsymbol{G}_n, \tag{2.1.29}$$

where $\boldsymbol{G}_n$, as above, maps $\boldsymbol{\mu}$ (resp. $\boldsymbol{m}$) into the Gauss rule $\boldsymbol{\gamma}$, and $\boldsymbol{H}_n$ maps the Gauss rule into the recursion coefficients,

$$\boldsymbol{H}_n : \ \mathbb{R}^{2n} \to \mathbb{R}^{2n} \quad \boldsymbol{\gamma} \mapsto \boldsymbol{\rho}. \tag{2.1.30}$$

Since, as will be seen later in §3.1.1, the map $\boldsymbol{H}_n$ is generally well-conditioned, the condition of $\boldsymbol{K}_n$ is more or less the same as the condition of $\boldsymbol{G}_n$. Hence, we will often consider the latter instead of the former.

2.1.4 *Condition of* $\boldsymbol{G}_n : \ \boldsymbol{\mu} \mapsto \boldsymbol{\gamma}$

Let n be a fixed, but arbitrary, integer ≥ 1 and the measure $\mathrm{d}\lambda$ positive definite on $\mathbb{P}$. Then $\Delta_n > 0$ by Theorem 1.2, and Theorem 2.1 shows that $\pi_n(\,\cdot\,;\mathrm{d}\lambda)$ exists and depends continuously and regularly on the moments μ_r, $r = 0, 1, \ldots, 2n-1$, in a neighborhood of the given moment vector $\boldsymbol{\mu}(\mathrm{d}\lambda)$. The same is true, therefore, of the zeros τ_ν of π_n, that is, of the Gaussian nodes, and also of the Gaussian weights λ_ν in view of (1.4.5) and (1.4.4). It makes sense, therefore, to talk about the condition of the map $\boldsymbol{G}_n : \ \boldsymbol{\mu} \mapsto \boldsymbol{\gamma}$ at $\boldsymbol{\mu} = \boldsymbol{\mu}(\mathrm{d}\lambda)$.

We begin by considering the absolute condition number of Definition 2.5,

$$(\operatorname{cond} \boldsymbol{G}_n)(\boldsymbol{\mu}) = \left\| \frac{\partial \boldsymbol{G}_n(\boldsymbol{\mu})}{\partial \boldsymbol{\mu}} \right\|,$$

where $\|\cdot\|$ is the infinity norm (2.1.14). Since the Gauss quadrature formula is exact on $\mathbb{P}_{2n-1}$, there holds

$$\sum_{\nu=1}^{n} \lambda_\nu \tau_\nu^r = \mu_r, \quad r = 0, 1, \ldots, 2n-1. \tag{2.1.31}$$

The map $\boldsymbol{G}_n$, therefore, amounts to solving the nonlinear system (2.1.31) for $\lambda_1, \ldots, \lambda_n, \tau_1, \ldots, \tau_n$. (The system is actually linear in the λs.) If $\boldsymbol{F}_n$ denotes the map $\boldsymbol{\gamma} \mapsto \boldsymbol{\mu}$ defined by (2.1.31), then by an elementary computation

$$\frac{\partial \boldsymbol{F}_n}{\partial \boldsymbol{\gamma}} = \boldsymbol{T}\boldsymbol{\Lambda},$$

where $\boldsymbol{\Lambda} \in \mathbb{R}^{2n \times 2n}$ is the diagonal matrix

$$\boldsymbol{\Lambda} = \operatorname{diag}(1, \ldots, 1, \lambda_1, \ldots, \lambda_n) \tag{2.1.32}$$

and $\boldsymbol{T}$ a confluent Vandermonde matrix

$$\boldsymbol{T} = \begin{bmatrix} 1 & \cdots & 1 & 0 & \cdots & 0 \\ \tau_1 & \cdots & \tau_n & 1 & \cdots & 1 \\ \tau_1^2 & \cdots & \tau_n^2 & 2\tau_1 & \cdots & 2\tau_n \\ \vdots & & \vdots & \vdots & & \vdots \\ \tau_1^{2n-1} & \cdots & \tau_n^{2n-1} & (2n-1)\tau_1^{2n-2} & \cdots & (2n-1)\tau_n^{2n-2} \end{bmatrix}. \tag{2.1.33}$$

Since the map $\boldsymbol{G}_n$ is the inverse of $\boldsymbol{F}_n$, one has

$$\frac{\partial \boldsymbol{G}_n}{\partial \boldsymbol{\mu}} = \left(\frac{\partial \boldsymbol{F}_n}{\partial \boldsymbol{\gamma}} \right)^{-1} = \boldsymbol{\Lambda}^{-1} \boldsymbol{T}^{-1}, \tag{2.1.34}$$

and thus

$$(\operatorname{cond} \boldsymbol{G}_n)(\boldsymbol{\mu}) = \| \boldsymbol{\Lambda}^{-1} \boldsymbol{T}^{-1} \|. \tag{2.1.35}$$

A lower bound of the condition number (2.1.35) can be found if one assumes that the measure $\mathrm{d}\lambda$ has support contained in the positive real line $\mathbb{R}_+$.

Theorem 2.11 *Let $\mathrm{d}\lambda$ be a positive definite measure having support in $\mathbb{R}_+$ and let $\pi_n(\,\cdot\,) = \pi_n(\,\cdot\,; \mathrm{d}\lambda)$ be the monic polynomial of degree n orthogonal with respect to $\mathrm{d}\lambda$. Then, the absolute condition number (2.1.35) satisfies*

$$(\operatorname{cond} \boldsymbol{G}_n)(\boldsymbol{\mu}) \geq \min \left(1, \frac{1}{\max_\nu \lambda_\nu} \right) \cdot \frac{[\pi_n(-1)]^2}{\min\limits_{1 \leq \nu \leq n} \{ (1+\tau_\nu) [\pi_n'(\tau_\nu)]^2 \}}, \tag{2.1.36}$$

where λ_ν and τ_ν are the weights and nodes of the n-point Gauss quadrature rule (1.4.7).

Proof Recalling that $\lambda_\nu > 0$ (cf. Theorem 1.46), we have from (2.1.35) that

$$(\operatorname{cond} \boldsymbol{G}_n)(\boldsymbol{\mu}) \geq \min \left(1, \frac{1}{\max_\nu \lambda_\nu} \right) \| \boldsymbol{T}^{-1} \|. \tag{2.1.37}$$

The infinity norm of $\boldsymbol{T}^{-1}$ has been studied in Gautschi (1963) and further estimated in Gautschi (1968). In particular, it has been shown (Gautschi, 1968, Theorem 2.1) that

$$\| \boldsymbol{T}^{-1} \| \geq \max_{1 \leq \nu \leq n} \left\{ (1+\tau_\nu) \prod_{\substack{\mu=1 \\ \mu \neq \nu}}^{n} \left(\frac{1+\tau_\mu}{\tau_\nu - \tau_\mu} \right)^2 \right\}.$$

Writing the expression in curled brackets in the form

$$\frac{\prod_{\mu=1}^n (1+\tau_\mu)^2}{(1+\tau_\nu) \prod_{\mu \neq \nu} (\tau_\nu - \tau_\mu)^2}$$

and noting from $\pi_n(t) = \prod_{\mu=1}^n (t - \tau_\mu)$ that $\pi_n(-1) = (-1)^n \prod_{\mu=1}^n (1+\tau_\mu)$ and $\pi_n'(\tau_\nu) = \prod_{\mu \neq \nu} (\tau_\nu - \tau_\mu)$ yields

$$\| \boldsymbol{T}^{-1} \| \geq \frac{[\pi_n(-1)]^2}{\min\limits_{1 \leq \nu \leq n} \{ (1+\tau_\nu) [\pi_n'(\tau_\nu)]^2 \}}.$$

Together with (2.1.37), this proves the theorem. □

The lower bound in (2.1.36) is computed by the `OPQ` routine `acondGlow.m`.

Remark to Theorem 2.11 The bound in (2.1.36) remains unchanged if π_n is multiplied by any constant c_n, and hence does not depend on the particular normalization of the orthogonal polynomial.

Example 2.12 *Chebyshev measure* on $[0,1]$.

Here, $\mathrm{d}\lambda(t) = [t(1-t)]^{-1/2}\,\mathrm{d}t$ and, taking advantage of the Remark to Theorem 2.11, one can take $\pi_n(t) = T_n(2t-1)$. Then,

$$[\pi_n(-1)]^2 = [T_n(-3)]^2 = [T_n(3)]^2, \tag{2.1.38}$$

and since (cf. (1.4.17))

$$\tau_\nu = \tfrac{1}{2}(1+\cos\theta_\nu), \quad \theta_\nu = \frac{2\nu-1}{2n}\,\pi, \tag{2.1.39}$$

one has

$$\pi_n'(\tau_\nu) = 2T_n'(2\tau_\nu - 1) = 2T_n'(\cos\theta_\nu).$$

Differentiating the identity $T_n(\cos\theta) = \cos n\theta$ (see (1.5.2)) gives $T_n'(\cos\theta) = n\sin n\theta/\sin\theta$, and thus

$$(1+\tau_\nu)[\pi_n'(\tau_\nu)]^2 = (\tfrac{3}{2} + \tfrac{1}{2}\cos\theta_\nu)\cdot 4n^2\left(\frac{\sin n\theta_\nu}{\sin\theta_\nu}\right)^2.$$

The minimum of this expression taken over $\nu = 1, 2, \ldots, n$ is less than, or equal to, its value at any fixed $\nu = \nu_0$. Taking $\nu_0 = \lfloor \frac{n}{2} \rfloor + 1$, hence $\sin n\theta_{\nu_0} = (-1)^{\nu_0}$, and $\cos\theta_{\nu_0} = 0$, $\sin\theta_{\nu_0} = 1$ if n is odd, $\cos\theta_{\nu_0} = -\sin(\pi/2n)$, $\sin\theta_{\nu_0} = \cos(\pi/2n)$ if n is even, one finds, using $\cos(\pi/2n) \geq 1/\sqrt{2}$ for $n \geq 2$, that

$$\min_\nu\{(1+\tau_\nu)[\pi_n'(\tau_\nu)]^2\} \leq (1+\tau_{\nu_0})[\pi_n'(\tau_{\nu_0})]^2 \leq 12n^2, \quad n \geq 2. \tag{2.1.40}$$

Moreover, $\lambda_\nu = \pi/n$ (cf. (1.4.20), transformed to the interval $[0,1]$), so that $\lambda_\nu < 1$ if $n \geq 4$, and thus

$$\min\left(1, \frac{1}{\max_\nu \lambda_\nu}\right) = 1, \quad n \geq 4. \tag{2.1.41}$$

Combining (2.1.38), (2.1.40), and (2.1.41) in (2.1.36) yields

$$(\operatorname{cond} \boldsymbol{G}_n)(\boldsymbol{\mu}) \geq \frac{[T_n(3)]^2}{12n^2}, \quad n \geq 4. \tag{2.1.42}$$

A more quantitative bound can be obtained by noting that $y_k = T_k(3)$ satisfies (see (1.5.8))

$$y_{k+1} - 6y_k + y_{k-1} = 0, \quad y_0 = 1,\ y_1 = 3,$$

so that from the theory of linear difference equations with constant coefficients,

$$y_n = T_n(3) = \tfrac{1}{2}\,(t_1^n + t_2^n)\,, \quad t_1 = 3 + \sqrt{8},\ t_2 = 3 - \sqrt{8}.$$

There follows $T_n(3) > \frac{1}{2} t_1^n$, and thus, from (2.1.42),

$$(\operatorname{cond} \boldsymbol{G}_n)(\boldsymbol{\mu}) > \frac{(17 + 6\sqrt{8})^n}{48n^2}\,, \quad n \geq 4. \tag{2.1.43}$$

It is seen that the condition number grows exponentially fast with n, at the rate $\exp[n \ln(17 + 6\sqrt{8})] = \exp(3.52549\ldots n)$, which, incidentally, coincides with the rate of growth of the (Turing) condition number for the nth-order segment of the Hilbert matrix as estimated by Todd (1954).

Although Example 2.12 may appear to be rather special, it is actually indicative of a much wider class of measures (supported on $[0, 1]$), the so-called Szegö class (cf. (1.3.10)), for which it is known that the Gauss nodes $\tau_\nu = \tau_\nu^G$ as $n \to \infty$ indeed assume the arccos-distribution of (2.1.39).

For measures supported on an infinite interval, which are likely to have moments μ_r that grow rapidly, a relative condition number, for example (2.1.17), may be more appropriate. Simple results such as (2.1.36) then no longer exist, but in turn, no assumptions are required on the support of $\mathrm{d}\lambda$. Applied to the map $\boldsymbol{G}_n(\boldsymbol{\mu})$, and using the mollified condition number of (2.1.18), one obtains

Theorem 2.13 *Let* $\mathrm{d}\lambda$ *be a positive measure. Then, the relative condition number of* $\boldsymbol{G}_n(\boldsymbol{\mu})$*, according to (2.1.17) and (2.1.18), is given by*

$$(\operatorname{cond} \boldsymbol{G}_n)(\boldsymbol{\mu}) = \|\boldsymbol{C}(\boldsymbol{\mu})\|, \tag{2.1.44}$$

where

$$\boldsymbol{C}(\boldsymbol{\mu}) = [c_{\kappa\lambda}(\boldsymbol{\mu})]_{\kappa,\lambda=1}^{2n},$$

and

$$c_{\kappa\lambda}(\boldsymbol{\mu}) = \frac{m(\mu_{\lambda-1})(\boldsymbol{T}^{-1})_{\kappa\lambda}}{m(\lambda_\kappa)}\,, \quad c_{n+\kappa,\lambda}(\boldsymbol{\mu}) = \frac{m(\mu_{\lambda-1})(\boldsymbol{T}^{-1})_{n+\kappa,\lambda}}{\lambda_\kappa m(\tau_\kappa)}\,, \tag{2.1.45}$$
$$\kappa = 1, 2, \ldots, n;\ \lambda = 1, 2, \ldots, 2n.$$

Here, $(\boldsymbol{T}^{-1})_{rs}$ *denotes the element of* $\boldsymbol{T}^{-1}$ *in row* r *and column* s *and* $m(\,\cdot\,)$ *is the mollifier function (2.1.11).*

The elements of $\boldsymbol{T}^{-1}$ are computed by the `OPQ` routine `Tinv.m`, and the relative condition number (2.1.44), in the infinity norm, by `rcondG.m` with `iopt` = 1.

The simpler, but more global, relative condition number (2.1.19) applied to the map $\boldsymbol{G}_n$, when using infinity norms, takes the form

$$(\operatorname{cond} \boldsymbol{G}_n)(\boldsymbol{\mu}) = \frac{\|\boldsymbol{\mu}\|_\infty \|\boldsymbol{\Lambda}^{-1}\boldsymbol{T}^{-1}\|_\infty}{\|\boldsymbol{\gamma}\|_\infty}\,. \tag{2.1.46}$$

It is computed by the `OPQ` routine `gcondG.m`.

It is interesting to compare the theoretical condition numbers with error magnifications observed numerically. We do this by applying the Chebyshev algorithm of §2.1.7, which actually implements the map $\boldsymbol{K}_n : \boldsymbol{\mu} \mapsto \boldsymbol{\rho}$, but whose condition is similar to the one of $\boldsymbol{G}_n$; cf. the remark at the end of §2.1.3. By "error magnification" we mean the absolute value of the observed error divided by the machine precision, where "error" is a "mollified" error, that is, the absolute error if the respective quantity is less than 1 in modulus, and the relative error otherwise. We illustrate this for the Legendre, Laguerre, and Hermite measures, using the `OPQ` routines `Table2_1.m`, `Table2_2.m`, and `Table2_3.m`.

Example 2.14 *Legendre measure* $\mathrm{d}\lambda(t) = \mathrm{d}t$ on $[0, 1]$.

The moments $\mu_r = 1/(r+1)$, $r = 0, 1, 2, \ldots$, are between 0 and 1, and the same is true for the nodes τ_ν and weights λ_ν of the Gauss quadrature rule. Therefore, both absolute and mollified relative condition numbers, and even the simplified condition number in (2.1.46), are appropriate. The three columns after the first in Table 2.1 display the lower bound of the condition number in (2.1.36), the infinity norm of the condition matrix in (2.1.44), and the simplified condition number in (2.1.46), for $n = 2, 5, 8, 11, 14$. The remaining two columns show the maximum observed error magnifications $\operatorname{mag}\alpha$ and $\operatorname{mag}\beta$ in the coefficients α_k resp. β_k, $k = 0, 1, \ldots, n-1$.

Table 2.1 *Condition number and error magnification for Legendre measure on* $[0, 1]$.

n	(2.1.36)	(2.1.44)	(2.1.46)	$\operatorname{mag}\alpha$	$\operatorname{mag}\beta$
2	1.16(1)	3.17(1)	4.02(1)	2.00(0)	6.25(–2)
5	1.34(5)	4.72(5)	4.95(5)	3.32(3)	5.04(2)
8	2.20(9)	1.21(10)	1.24(10)	2.77(8)	1.30(6)
11	4.62(13)	3.45(14)	3.48(14)	8.33(12)	5.50(11)
14	1.15(18)	1.07(19)	1.08(19)	4.85(16)	4.31(17)

It can be seen that all three condition numbers grow very rapidly, the first, being a lower bound, at a slightly slower rate. The simplified condition number (2.1.46), in this example, is practically identical with the more detailed condition number in (2.1.44). The actually observed error magnifications exhibit the same trend of rapid growth, but are generally a few orders of magnitude smaller than predicted, and this in spite of additional errors committed during the execution of the algorithm. The reason for this seems to be a certain amount of internal cancellation of errors.

Example 2.15 *Generalized Laguerre measure* $\mathrm{d}\lambda(t) = t^\alpha \mathrm{e}^{-t}\,\mathrm{d}t$ on $[0, \infty]$ with $\alpha = -\frac{1}{2}$.

The case $\alpha = 0$ of ordinary Laguerre measures would be atypical inasmuch as Matlab produces exact integer results, at least up to $n = 11$, and hence zero errors. This is not so for nonzero α, say $\alpha = -\frac{1}{2}$.

Here, the moments $\mu_r = \Gamma(\alpha + r + 1)$, $r = 0, 1, 2, \ldots$, grow very rapidly, so

that the absolute condition number in (2.1.36) is inappropriate and (2.1.46) is likely to be too pessimistic. This is confirmed in Table 2.2 giving information

Table 2.2 *Condition number and error magnification for Laguerre measure with parameter* $\alpha = 0.5$.

n	(2.1.36)	(2.1.44)	(2.1.46)	mag α	mag β
2	1.83(0)	3.62(0)	7.57(0)	8.00(–1)	2.50(–1)
5	2.62(1)	1.25(3)	1.20(6)	3.36(2)	2.37(2)
8	2.32(2)	4.32(5)	1.52(13)	2.19(6)	7.77(5)
11	1.16(3)	2.10(8)	2.01(21)	3.03(9)	2.36(9)
14	4.61(3)	1.10(11)	1.36(30)	4.47(11)	2.26(11)

analogous to that in Table 2.1: the column headed by (2.1.36) has little to do with the actual error magnifications in the last two columns, and the one headed (2.1.46) is grossly misleading, overestimating the error growth by many orders of magnitude, especially when n is large. The relative condition number in (2.1.44), on the other hand, predicts the error magnification rather accurately.

Example 2.16 *Hermite measure* $\mathrm{d}\lambda(t) = \mathrm{e}^{-t^2}\,\mathrm{d}t$ on $\mathbb{R}$.

While the moments μ_r for r odd are zero, those for even r are $\Gamma((r+1)/2)$ and as in Example 2.15 grow rapidly. Not only is the absolute condition number in (2.1.36) inappropriate, but the lower bound in fact is not even applicable. As can be seen from Table 2.3, no errors have been observed in the αs, which are all zero, and the error magnification in the βs is more or less as predicted by (2.1.44), but decidedly lower than in Example 2.15. As in the previous example, the condition number (2.1.46) is not a reliable indicator of error growth.

Table 2.3 *Condition number and error magnification for Hermite measure.*

n	(2.1.36)	(2.1.44)	(2.1.46)	mag α	mag β
2	—	2.65(0)	4.54(0)	0	0.00(0)
5	—	1.07(1)	4.20(1)	0	1.33(0)
8	—	9.97(1)	2.21(4)	0	6.57(1)
11	—	1.51(3)	3.36(7)	0	2.21(3)
14	—	2.88(4)	1.28(11)	0	1.50(5)

2.1.5 *Condition of* $\boldsymbol{G}_n : \boldsymbol{m} \mapsto \boldsymbol{\gamma}$

As was already mentioned at the beginning of §2.1, modified moments can be expected to yield maps $\boldsymbol{G}_n$ that are better conditioned. This will now be analyzed in the case where modified moments are defined in terms of monic polynomials $p_k(\,\cdot\,) = p_k(\,\cdot\,;\mathrm{d}\ell)$ orthogonal with respect to a positive measure $\mathrm{d}\ell$ (cf. Example 2.8). The support of $\mathrm{d}\ell$ may be bounded or unbounded, and need not necessarily coincide with the support of the given measure $\mathrm{d}\lambda$. (See, however, the remarks

after the proof of Theorem 2.17.) All moments of $\mathrm{d}\ell$ are assumed to exist.

It will be convenient to consider the slightly modified map

$$\widetilde{\boldsymbol{G}}_n : \ \mathbb{R}^{2n} \to \mathbb{R}^{2n} \quad \widetilde{\boldsymbol{m}} \mapsto \boldsymbol{\gamma}, \tag{2.1.47}$$

where $\widetilde{\boldsymbol{m}} = [\widetilde{m}_0, \widetilde{m}_1, \ldots, \widetilde{m}_{2n-1}]^{\mathrm{T}}$ is the vector of *normalized* modified moments

$$\widetilde{m}_k = \frac{1}{\sqrt{d_k}}\, m_k, \quad d_k = \int_{\mathbb{R}} p_k^2(t)\, \mathrm{d}\ell(t), \quad k = 0, 1, \ldots, 2n-1, \tag{2.1.48}$$

with m_k as defined in (2.1.23). This has the theoretical advantage of making the $\widetilde{m}_k$ independent of the normalization of the orthogonal polynomials $\{p_k\}$. For algorithmic purposes, however, the passage from $\boldsymbol{m}$ to $\widetilde{\boldsymbol{m}}$ is not required, and in fact not recommended; cf. §2.1.7. The additional diagonal map introduced, $\boldsymbol{D}_n : \ \boldsymbol{m} \mapsto \widetilde{\boldsymbol{m}}$, of course, is harmless, since each individual transformation $m_k \mapsto \widetilde{m}_k$ involves just one multiplication and is therefore perfectly well-conditioned.

We study the condition of $\widetilde{\boldsymbol{G}}_n$ in terms of the Frobenius matrix norm $\| \cdot \|_F$.

With $\tau_\nu = \tau_\nu(\mathrm{d}\lambda)$ and $\lambda_\nu = \lambda_\nu(\mathrm{d}\lambda)$ denoting the nodes and weights of the Gauss quadrature rule (1.4.7), we denote by h_ν and k_ν, as in (1.4.13), the elementary Hermite interpolation polynomials associated with the nodes $\tau_1, \ldots, \tau_n$, which satisfy

$$\begin{aligned} &h_\nu(\tau_\mu) = \delta_{\nu\mu}, \quad h_\nu'(\tau_\mu) = 0, \\ &k_\nu(\tau_\mu) = 0, \quad k_\nu'(\tau_\mu) = \delta_{\nu\mu}, \end{aligned} \qquad \nu, \mu = 1, 2, \ldots, n. \tag{2.1.49}$$

Theorem 2.17 *The absolute condition number of the map $\widetilde{\boldsymbol{G}}_n$, in the sense of Definition 2.5, with $\| \cdot \|$ the Frobenius norm, is given by*

$$(\operatorname{cond} \widetilde{\boldsymbol{G}}_n)(\widetilde{\boldsymbol{m}}) = \left\{ \int_{\mathbb{R}} g_n(t; \mathrm{d}\lambda)\, \mathrm{d}\ell(t) \right\}^{1/2}, \tag{2.1.50}$$

where

$$g_n(t; \mathrm{d}\lambda) = \sum_{\nu=1}^{n} \left(h_\nu^2(t) + \frac{1}{\lambda_\nu^2}\, k_\nu^2(t) \right) \tag{2.1.51}$$

and h_ν, k_ν are the elementary Hermite interpolation polynomials (1.4.13) associated with the Gaussian nodes $\tau_1, \ldots, \tau_n$.

Proof The map $\widetilde{\boldsymbol{G}}_n : \ \widetilde{\boldsymbol{m}} \mapsto \boldsymbol{\gamma}$, similarly as in (2.1.31), amounts to solving the system of nonlinear equations

$$\frac{1}{\sqrt{d_k}} \sum_{\nu=1}^{n} \lambda_\nu p_k(\tau_\nu) = \widetilde{m}_k, \quad k = 0, 1, \ldots, 2n-1. \tag{2.1.52}$$

If $\widetilde{\boldsymbol{F}}_n$ denotes the map $\boldsymbol{\gamma} \mapsto \widetilde{\boldsymbol{m}}$ defined by (2.1.52), it is elementary to show that

$$\frac{\partial \widetilde{\boldsymbol{F}}_n}{\partial \boldsymbol{\gamma}} = \boldsymbol{D}^{-1}\boldsymbol{P}\boldsymbol{\Lambda}, \tag{2.1.53}$$

where $\boldsymbol{D}$ and $\boldsymbol{\Lambda}$ are diagonal matrices of order $2n$,

$$\boldsymbol{D} = \operatorname{diag}(\sqrt{d_0}, \sqrt{d_1}, \ldots, \sqrt{d_{2n-1}}), \quad \boldsymbol{\Lambda} = \operatorname{diag}(1, \ldots, 1, \lambda_1, \ldots, \lambda_n)$$

and

$$\boldsymbol{P} = \begin{bmatrix} p_0(\tau_1) & \cdots & p_0(\tau_n) & p_0'(\tau_1) & \cdots & p_0'(\tau_n) \\ p_1(\tau_1) & \cdots & p_1(\tau_n) & p_1'(\tau_1) & \cdots & p_1'(\tau_n) \\ \vdots & & \vdots & \vdots & & \vdots \\ p_{2n-1}(\tau_1) & \cdots & p_{2n-1}(\tau_n) & p_{2n-1}'(\tau_1) & \cdots & p_{2n-1}'(\tau_n) \end{bmatrix}. \tag{2.1.54}$$

Therefore, noting that $\widetilde{\boldsymbol{G}}_n$ is the inverse map of $\widetilde{\boldsymbol{F}}_n$, one has

$$\frac{\partial \widetilde{\boldsymbol{G}}_n}{\partial \widetilde{\boldsymbol{m}}} = \left(\frac{\partial \widetilde{\boldsymbol{F}}_n}{\partial \boldsymbol{\gamma}}\right)^{-1} = \boldsymbol{\Lambda}^{-1}\boldsymbol{P}^{-1}\boldsymbol{D} \tag{2.1.55}$$

and, thus,

$$(\operatorname{cond} \widetilde{\boldsymbol{G}}_n)(\widetilde{\boldsymbol{m}}) = \|\boldsymbol{\Lambda}^{-1}\boldsymbol{P}^{-1}\boldsymbol{D}\|_F. \tag{2.1.56}$$

The principal issue at hand is the inversion of matrix $\boldsymbol{P}$ in (2.1.54). To accomplish this, we expand the Hermite polynomials h_ν and k_ν in the orthogonal polynomials $\{p_k\}$,

$$h_\nu(t) = \sum_{\mu=1}^{2n} a_{\nu\mu} p_{\mu-1}(t), \quad k_\nu(t) = \sum_{\mu=1}^{2n} b_{\nu\mu} p_{\mu-1}(t), \tag{2.1.57}$$

and solve the system of linear equations

$$\sum_{\lambda=1}^{n} \{p_{\mu-1}(\tau_\lambda) u_\lambda + p_{\mu-1}'(\tau_\lambda) u_{n+\lambda}\} = v_\mu, \quad \mu = 1, 2, \ldots, 2n,$$

whose coefficient matrix is $\boldsymbol{P}$. Multiplying the μth equation by $a_{\nu\mu}$ and adding over $\mu = 1, 2, \ldots, 2n$, one obtains, in view of the first of (2.1.57) and (2.1.49),

$$u_\nu = \sum_{\mu=1}^{2n} a_{\nu\mu} v_\mu, \quad \nu = 1, 2, \ldots, n.$$

Similarly, multiplying the μth equation by $b_{\nu\mu}$ and adding yields

$$u_{n+\nu} = \sum_{\mu=1}^{2n} b_{\nu\mu} v_\mu, \quad \nu = 1, 2, \ldots, n.$$

There follows

$$\boldsymbol{P}^{-1} = \begin{bmatrix} \boldsymbol{A} \\ \boldsymbol{B} \end{bmatrix}, \quad \boldsymbol{A} = [a_{\nu\mu}], \quad \boldsymbol{B} = [b_{\nu\mu}]. \tag{2.1.58}$$

Since

$$(\boldsymbol{\Lambda}^{-1}\boldsymbol{P}^{-1}\boldsymbol{D})_{\nu\mu} = \sqrt{d_{\mu-1}}a_{\nu\mu}, \ (\boldsymbol{\Lambda}^{-1}\boldsymbol{P}^{-1}\boldsymbol{D})_{n+\nu,\mu} = \frac{1}{\lambda_\nu}\sqrt{d_{\mu-1}}b_{\nu\mu}, \ \nu = 1, \dots, n, \tag{2.1.59}$$

one obtains

$$\|\boldsymbol{\Lambda}^{-1}\boldsymbol{P}^{-1}\boldsymbol{D}\|_F^2 = \sum_{\nu=1}^{n}\sum_{\mu=1}^{2n} d_{\mu-1}\left(a_{\nu\mu}^2 + \frac{1}{\lambda_\nu^2}b_{\nu\mu}^2\right). \tag{2.1.60}$$

On the other hand,

$$\begin{aligned}\int_{\mathbb{R}} h_\nu^2(t)\,\mathrm{d}\ell(t) &= \int_{\mathbb{R}} \sum_{\mu=1}^{2n} a_{\nu\mu}p_{\mu-1}(t) \sum_{\kappa=1}^{2n} a_{\nu\kappa}p_{\kappa-1}(t)\,\mathrm{d}\ell(t) \\ &= \sum_{\mu,\kappa=1}^{2n} a_{\nu\mu}a_{\nu\kappa}\int_{\mathbb{R}} p_{\mu-1}(t)p_{\kappa-1}(t)\,\mathrm{d}\ell(t) \\ &= \sum_{\mu=1}^{2n} d_{\mu-1}a_{\nu\mu}^2\end{aligned}$$

by virtue of the orthogonality of the p_k. Similarly,

$$\int_{\mathbb{R}} k_\nu^2(t)\,\mathrm{d}\ell(t) = \sum_{\mu=1}^{2n} d_{\mu-1}b_{\nu\mu}^2.$$

Therefore,

$$\|\boldsymbol{\Lambda}^{-1}\boldsymbol{P}^{-1}\boldsymbol{D}\|_F^2 = \int_{\mathbb{R}} \sum_{\nu=1}^{n}\left(h_\nu^2(t) + \frac{1}{\lambda_\nu^2}k_\nu^2(t)\right)\mathrm{d}\ell(t),$$

which in view of (2.1.56) and (2.1.51) proves the theorem. □

Theorem 2.17 shows clearly how, for given n, the absolute condition of $\widetilde{\boldsymbol{G}}_n$ depends on the two measures, $\mathrm{d}\lambda$ and $\mathrm{d}\ell$, involved. The dependence on $\mathrm{d}\lambda$ manifests itself entirely through the Gaussian nodes and weights $\tau_\nu = \tau_\nu(\mathrm{d}\lambda)$ and $\lambda_\nu = \lambda_\nu(\mathrm{d}\lambda)$, belonging to the measure $\mathrm{d}\lambda$, the former of which uniquely determine the Hermite polynomials h_ν and k_ν. The influence of $\mathrm{d}\ell$ is usually weaker inasmuch as this measure only plays a role as an integration measure in the integral on the right of (2.1.50).

The polynomial $g_n(\,\cdot\,) = g_n(\,\cdot\,;\mathrm{d}\lambda)$ has some noteworthy properties: it trivially is positive,

$$g_n(t) > 0 \quad \text{on } \mathbb{R}, \tag{2.1.61}$$

and it satisfies

$$g_n(\tau_\nu) = 1, \quad g_n'(\tau_\nu) = 0, \quad \nu = 1, 2, \ldots, n, \tag{2.1.62}$$

as follows immediately from (2.1.49). These properties suggest that g_n cannot deviate too much from 1 on the support of $\mathrm{d}\lambda$, especially if the latter is a finite interval and the nodes τ_ν have an arccos-distribution on that interval. (For equally spaced τ_ν, the polynomial g_n could well exhibit large oscillations reminiscent of those occurring in Lagrange interpolation.) Since g_n outside the support of $\mathrm{d}\lambda$ grows very rapidly, it is prudent to choose $\mathrm{d}\ell$ to have its support contained in, or identical with, that of $\mathrm{d}\lambda$. For large classes of measures with compact support, it is in fact necessary to have $\mathrm{supp}(\mathrm{d}\ell)$=$\mathrm{supp}(\mathrm{d}\lambda)$ if exponential growth of the condition number is to be avoided; see Beckermann and Bourreau (1998, Theorem 11).

In Gautschi (1986), a distinction is made between *weak* and *strong* nodes τ_ν, for which $g_n''(\tau_\nu) < 0$ resp. $g_n''(\tau_\nu) > 0$. Between consecutive weak nodes, g_n very likely (though not necessarily) remains < 1, whereas in the neighborhood of a strong node, g_n assumes values larger, and potentially very much larger, than 1 on either side. It is also very likely that between consecutive strong nodes g_n remains > 1.

An elementary computation based on (1.4.13) and (2.1.51) will show that

$$\begin{aligned} \frac{1}{2} g_n''(\tau_\nu) &= 2\ell_\nu''(\tau_\nu) - 6[\ell_\nu'(\tau_\nu)]^2 + \frac{1}{\lambda_\nu^2} \\ &= 2 \sum_{k \neq \nu} \sum_{\substack{\ell \neq \nu \\ \ell \neq k}} \frac{1}{(\tau_\nu - \tau_k)(\tau_\nu - \tau_\ell)} - 6 \left(\sum_{k \neq \nu} \frac{1}{\tau_\nu - \tau_k} \right)^2 + \frac{1}{\lambda_\nu^2}\,. \end{aligned} \tag{2.1.63}$$

The node τ_ν, therefore, is weak or strong depending on whether the expression on the right of (2.1.63) is negative or positive.

Example 2.18 Chebyshev nodes $\tau_\nu = \cos\theta_\nu$, $\theta_\nu = (2\nu-1)\pi/2n$, $\nu = 1, 2, \ldots, n$.

These, for each $n = 2, 3, \ldots$, on the basis of (2.1.63) turn out to be all weak nodes (Gautschi, 1986, Theorem 4.1). In this case, $g_n(t)$ indeed is ≤ 1 for all $-1 \leq t \leq 1$; cf. Example 2.20.

Theorem 2.19 *The relative condition number of $\widetilde{\boldsymbol{G}}_n(\widetilde{\boldsymbol{m}})$, according to (2.1.17) and (2.1.18), is given by*

$$(\mathrm{cond}\, \widetilde{\boldsymbol{G}}_n)(\widetilde{\boldsymbol{m}}) = \|\boldsymbol{C}(\widetilde{\boldsymbol{m}})\|, \tag{2.1.64}$$

where

$$\boldsymbol{C}(\widetilde{\boldsymbol{m}}) = [c_{\nu\mu}(\widetilde{\boldsymbol{m}})]_{\nu,\mu=1}^{2n}$$

and

$$c_{\nu\mu}(\widetilde{\boldsymbol{m}}) = \sqrt{d_{\mu-1}}\, \frac{m(\widetilde{m}_{\mu-1})|a_{\nu\mu}|}{m(\lambda_\nu)}\,, \quad c_{n+\nu,\mu}(\widetilde{\boldsymbol{m}}) = \sqrt{d_{\mu-1}}\, \frac{m(\widetilde{m}_{\mu-1})|b_{\nu\mu}|}{\lambda_\nu m(\tau_\nu)}\,, \quad \nu = 1, \ldots, n. \tag{2.1.65}$$

Here, $a_{\nu\mu}$ and $b_{\nu\mu}$ are the coefficients in the expansions (2.1.57) of h_ν and k_ν, $d_{\mu-1}$ the constants defined in (2.1.48), and $m(\,\cdot\,)$ is the mollifier function (2.1.11).

Proof The results (2.1.64) and (2.1.65) are immediate consequences of (2.1.55), (2.1.59), and (2.1.18). □

`OPQ` routines for the absolute condition number (2.1.50) and for the relative condition number in (2.1.64) are `acondG.m` and `rcondG.m`, respectively.

In order to compute the absolute condition number, note that g_n is a polynomial of degree $\leq 4n-2$, so that the integral in (2.1.50) can be evaluated exactly (up to rounding errors) by means of the $(2n)$-point Gauss quadrature rule associated with the measure $\mathrm{d}\ell$. This is unproblematic since $\mathrm{d}\ell$ is usually one of the classical integration measures and, besides, the integrand is positive. A similar remark applies to the evaluation of the quantities $a_{\nu\mu} = d_{\mu-1}^{-1} \int_{\mathbb{R}} h_\nu(t) p_{\mu-1}(t)\,\mathrm{d}\ell(t)$ and $b_{\nu\mu} = d_{\mu-1}^{-1} \int_{\mathbb{R}} k_\nu(t) p_{\mu-1}(t)\,\mathrm{d}\ell(t)$, which are needed to compute the relative condition number.

As regards the computation of the polynomials h_ν, k_ν, and g_n, recall from (1.4.13) that the former two are expressible in terms of the elementary Lagrange polynomials ℓ_ν of (1.4.4) and $\ell_\nu'(\tau_\nu)$, which in turn can be written as

$$\ell_\nu(t) = [(t-\tau_\nu)\rho_\nu]^{-1}\omega_n(t), \quad \ell_\nu'(\tau_\nu) = \sigma_\nu, \tag{2.1.66}$$

where $\omega_n(t) = \prod_{\kappa=1}^n (t-\tau_\kappa)$ and

$$\rho_\nu = \prod_{\substack{\mu=1\\ \mu\neq\nu}}^n (\tau_\nu - \tau_\mu), \quad \sigma_\nu = \sum_{\substack{\mu=1\\ \mu\neq\nu}}^n \frac{1}{\tau_\nu - \tau_\mu}\,. \tag{2.1.67}$$

Since

$$1 \equiv \sum_{\kappa=1}^n \ell_\kappa(t) = \left(\sum_{\kappa=1}^n \ell_\kappa(t)\right)^2 = \omega_n^2(t) \left(\sum_{\kappa=1}^n [(t-\tau_\kappa)\rho_\kappa]^{-1}\right)^2, \tag{2.1.68}$$

one gets from (1.4.13)

$$h_\nu(t) = (1-2(t-\tau_\nu)\sigma_\nu)\ell_\nu^2(t) = \frac{(1-2(t-\tau_\nu)\sigma_\nu)\ell_\nu^2(t)}{\left(\sum_{\kappa=1}^n \ell_\kappa(t)\right)^2},$$

and thus from (2.1.66) and (2.1.68),

$$h_\nu(t) = \frac{(1-2(t-\tau_\nu)\sigma_\nu)[(t-\tau_\nu)\rho_\nu]^{-2}}{\left(\sum_{\kappa=1}^n [(t-\tau_\kappa)\rho_\kappa]^{-1}\right)^2}\,. \tag{2.1.69}$$

Similarly,

$$k_\nu(t) = \frac{[(t-\tau_\nu)\rho_\nu]^{-2}(t-\tau_\nu)}{\left(\sum_{\kappa=1}^n [(t-\tau_\kappa)\rho_\kappa]^{-1}\right)^2}\,. \tag{2.1.70}$$

Using (2.1.69) and (2.1.70) finally yields

$$g_n(t) = \frac{\sum_{\nu=1}^{n}[(t-\tau_\nu)\rho_\nu]^{-4}\left((1-2(t-\tau_\nu)\sigma_\nu)^2 + \frac{1}{\lambda_\nu^2}(t-\tau_\nu)^2\right)}{\left(\sum_{\kappa=1}^{n}[(t-\tau_\kappa)\rho_\kappa]^{-1}\right)^4}. \tag{2.1.71}$$

The OPQ routine g_n.m computes $g_n(t)$ from the representation (2.1.71).

Example 2.20 *Chebyshev measure* $\mathrm{d}\lambda(t) = (1-t^2)^{-1/2}\,\mathrm{d}t$ on $[-1,1]$.

It was conjectured in Gautschi (1986, §4.1) and proved by Fischer (1998) that for all $n \geq 2$

$$g_n(t;\mathrm{d}\lambda) \leq 1 \quad \text{on } [-1,1]. \tag{2.1.72}$$

Theorem 2.17, in this case, implies that

$$(\operatorname{cond}\widetilde{\boldsymbol{G}}_n)(\widetilde{\boldsymbol{m}}) \leq \int_{\mathbb{R}} \mathrm{d}\ell(t), \quad n \geq 2, \tag{2.1.73}$$

provided the support of $\mathrm{d}\ell$ is contained in $[-1,1]$. Rather remarkably, the absolute condition of $\widetilde{\boldsymbol{G}}_n$ is uniformly bounded in n, and this regardless of the particular choice of $\mathrm{d}\ell$, that is, the particular choice of the modified moments.

2.1.6 *Condition of* $\boldsymbol{K}_n : \boldsymbol{m} \mapsto \boldsymbol{\rho}$

Although the map $\boldsymbol{K}_n$ can be expressed in terms of the map $\boldsymbol{G}_n$ via the composition (2.1.29) with a well-conditioned map $\boldsymbol{H}_n$, it is possible to analyze the condition of $\boldsymbol{K}_n$ directly, indeed for arbitrary modified moments as defined in §2.1.3.

Note, to begin with, that the first $2n$ modified moments

$$m_k = \int_{\mathbb{R}} p_k(t)\,\mathrm{d}\lambda(t), \quad k = 0,1,\ldots,2n-1, \tag{2.1.74}$$

are expressible linearly in terms of the first $2n$ ordinary moments, the matrix involved being nonsingular because of the p_k forming a basis of $\mathbb{P}_{2n-1}$ by assumption. Conversely, therefore, the first $2n$ ordinary moments are expressible as a nonsingular linear transformation of the first $2n$ modified moments. From (1.3.3) and (1.3.4), it can be seen that the recursion coefficients $\alpha_k = \alpha_k(\mathrm{d}\lambda)$, $\beta_k = \beta_k(\mathrm{d}\lambda)$, $k = 0,1,\ldots,n-1$, are rational functions of the first $2n$ ordinary moments, with positive denominator polynomials in some neighborhood of the given moments $\boldsymbol{\mu} = \boldsymbol{\mu}(\mathrm{d}\lambda)$. The same is, therefore, true for the modified moments. It thus makes sense to talk about the condition $(\operatorname{cond}\boldsymbol{K}_n)(\boldsymbol{m})$ of the map $\boldsymbol{K}_n : \boldsymbol{m} \mapsto \boldsymbol{\rho}$ at the given vector $\boldsymbol{m} = \boldsymbol{m}(\mathrm{d}\lambda)$ of modified moments.

Since $\{p_j\}_{j=0}^{2n-1}$ is a basis of $\mathbb{P}_{2n-1}$, every real polynomial $q \in \mathbb{P}_{2n-1}$ has a unique representation

$$q(t) = \sum_{j=0}^{2n-1} c_j[q]\,p_j(t) \tag{2.1.75}$$

in terms of the polynomials p_j, the coefficients $c_j[q]$ being linear continuous functionals $c_j : \mathbb{P}_{2n-1} \to \mathbb{R}$. In order to compute the Jacobian matrix $\partial\boldsymbol{K}_n/\partial\boldsymbol{m}$, the following lemma will be useful.

Lemma 2.21 *Let $q \in \mathbb{P}_{2n-1}$ be a polynomial which depends on the first $2n$ modified moments $m_0, m_1, \ldots, m_{2n-1}$ and has continuous partial derivatives in the neighborhood of some point $\boldsymbol{m} = [m_0, m_1, \ldots, m_{2n-1}]$. Then,*

$$\frac{\partial}{\partial m_k} \int_{\mathbb{R}} q(t)\, \mathrm{d}\lambda(t) = c_k[q] + \int_{\mathbb{R}} \frac{\partial q(t)}{\partial m_k}\, \mathrm{d}\lambda(t). \tag{2.1.76}$$

Proof From (2.1.75) one has

$$\int_{\mathbb{R}} q(t)\, \mathrm{d}\lambda(t) = \sum_{j=0}^{2n-1} c_j[q]\, m_j. \tag{2.1.77}$$

Differentiating with respect to m_k yields

$$\frac{\partial}{\partial m_k} \int_{\mathbb{R}} q(t)\, \mathrm{d}\lambda(t) = c_k[q] + \sum_{j=0}^{2n-1} \frac{\partial c_j[q]}{\partial m_k}\, m_j.$$

Since $c_j[\,\cdot\,]$ is a continuous linear functional, differentiation of the functional c_j with respect to m_k can be interchanged with the application of the functional to the derivative. Thus,

$$\begin{aligned} \frac{\partial}{\partial m_k} \int_{\mathbb{R}} q(t)\, \mathrm{d}\lambda(t) &= c_k[q] + \sum_{j=0}^{2n-1} c_j \left[\frac{\partial q}{\partial m_k}\right] m_j \\ &= c_k[q] + \int_{\mathbb{R}} \frac{\partial q(t)}{\partial m_k}\, \mathrm{d}\lambda(t), \end{aligned}$$

the last equation following from (2.1.77) with q replaced by $\partial q/\partial m_k$. This proves the lemma. □

Theorem 2.22 *Let $\tilde{\pi}_k(\,\cdot\,) = \tilde{\pi}_k(\,\cdot\,; \mathrm{d}\lambda)$ denote the orthonormal polynomials with respect to the measure* $\mathrm{d}\lambda$ (cf. §1.3.2). *Then,*

$$\frac{\partial \boldsymbol{K}_n}{\partial \boldsymbol{m}} = \begin{bmatrix} \dfrac{\partial \boldsymbol{\alpha}}{\partial \boldsymbol{m}} \\ \dfrac{\partial \boldsymbol{\beta}}{\partial \boldsymbol{m}} \end{bmatrix}, \quad \frac{\partial \boldsymbol{\alpha}}{\partial \boldsymbol{m}} = \left[\frac{\partial \alpha_j}{\partial m_k}\right] \in \mathbb{R}^{n \times 2n}, \quad \frac{\partial \boldsymbol{\beta}}{\partial \boldsymbol{m}} = \left[\frac{\partial \beta_j}{\partial m_k}\right] \in \mathbb{R}^{n \times 2n}, \tag{2.1.78}$$

where

$$\frac{\partial \alpha_j}{\partial m_k} = c_k[\tilde{\psi}_{2j+1}], \quad \frac{\partial \beta_j}{\partial m_k} = c_k[\tilde{\psi}_{2j}], \quad j = 0, 1, \ldots, n-1;\ k = 0, 1, \ldots, 2n-1, \tag{2.1.79}$$

and $\tilde{\psi}_0, \tilde{\psi}_1, \ldots, \tilde{\psi}_{2n-1}$ are polynomials defined by

$$\begin{aligned} \tilde{\psi}_{2j}(t) &= \beta_j \left(\tilde{\pi}_j^2(t) - \tilde{\pi}_{j-1}^2(t)\right), \\ \tilde{\psi}_{2j+1}(t) &= \sqrt{\beta_{j+1}}\tilde{\pi}_j(t)\tilde{\pi}_{j+1}(t) - \sqrt{\beta_j}\tilde{\pi}_{j-1}(t)\tilde{\pi}_j(t), \\ &\qquad\qquad j = 0, 1, \ldots, n-1, \end{aligned} \tag{2.1.80}$$

with $\tilde{\pi}_{-1}$ *and* β_0 *defined by* $\tilde{\pi}_{-1} = 0$ *resp.* $\beta_0 = \int_{\mathbb{R}} \mathrm{d}\lambda(t)$. (Note that $\tilde{\psi}_r$ is a polynomial of exact degree r for $r = 0, 1, \ldots, 2n-1$.)

Proof Differentiating the orthonormality relations

$$\int_{\mathbb{R}} \tilde{\pi}_i(t)\tilde{\pi}_j(t)\,\mathrm{d}\lambda(t) = 0 \quad (i < j), \qquad \int_{\mathbb{R}} \tilde{\pi}_j^2(t)\,\mathrm{d}\lambda(t) = 1 \tag{2.1.81}$$

with respect to m_k and using Lemma 2.21, one obtains from the first relation, for $i < j$,

$$\begin{aligned} 0 &= c_k[\tilde{\pi}_i\tilde{\pi}_j] + \int_{\mathbb{R}} \frac{\partial\tilde{\pi}_i(t)}{\partial m_k}\,\tilde{\pi}_j(t)\,\mathrm{d}\lambda(t) + \int_{\mathbb{R}} \tilde{\pi}_i(t)\frac{\partial\tilde{\pi}_j(t)}{\partial m_k}\,\mathrm{d}\lambda(t) \\ &= c_k[\tilde{\pi}_i\tilde{\pi}_j] + \int_{\mathbb{R}} \tilde{\pi}_i(t)\,\frac{\partial\tilde{\pi}_j(t)}{\partial m_k}\,\mathrm{d}\lambda(t), \end{aligned}$$

where the second equality follows from orthogonality. Thus,

$$\int_{\mathbb{R}} \tilde{\pi}_i(t)\,\frac{\partial\tilde{\pi}_j(t)}{\partial m_k}\,\mathrm{d}\lambda(t) = -c_k[\tilde{\pi}_i\tilde{\pi}_j], \quad i < j. \tag{2.1.82}$$

The second relation in (2.1.81), similarly, gives

$$0 = c_k[\tilde{\pi}_j^2] + 2\int_{\mathbb{R}} \tilde{\pi}_j(t)\,\frac{\partial\tilde{\pi}_j(t)}{\partial m_k}\,\mathrm{d}\lambda(t),$$

that is,

$$\int_{\mathbb{R}} \tilde{\pi}_j(t)\,\frac{\partial\tilde{\pi}_j(t)}{\partial m_k}\,\mathrm{d}\lambda(t) = -\tfrac{1}{2}c_k[\tilde{\pi}_j^2]. \tag{2.1.83}$$

Next, we differentiate the three-term recurrence relation (see (1.3.13))

$$\sqrt{\beta_{j+1}}\tilde{\pi}_{j+1}(t) = (t-\alpha_j)\tilde{\pi}_j(t) - \sqrt{\beta_j}\tilde{\pi}_{j-1}(t), \quad j = 0, 1, 2, \ldots, \tag{2.1.84}$$

with respect to m_k to get

$$\begin{aligned} &\frac{\partial\sqrt{\beta_{j+1}}}{\partial m_k}\,\tilde{\pi}_{j+1}(t) + \sqrt{\beta_{j+1}}\,\frac{\partial\tilde{\pi}_{j+1}(t)}{\partial m_k} \\ &= -\frac{\partial\alpha_j}{\partial m_k}\,\tilde{\pi}_j(t) + (t-\alpha_j)\,\frac{\partial\tilde{\pi}_j(t)}{\partial m_k} - \frac{\partial\sqrt{\beta_j}}{\partial m_k}\,\tilde{\pi}_{j-1}(t) - \sqrt{\beta_j}\,\frac{\partial\tilde{\pi}_{j-1}(t)}{\partial m_k}\,. \end{aligned} \tag{2.1.85}$$

To focus on the derivative of β_{j+1}, we multiply (2.1.85) by $\tilde{\pi}_{j+1}$ and integrate. Using (2.1.83) with j replaced by $j+1$ and orthonormality of the $\tilde{\pi}_k$, one finds

$$\frac{\partial\sqrt{\beta_{j+1}}}{\partial m_k} - \tfrac{1}{2}\sqrt{\beta_{j+1}}c_k[\tilde{\pi}_{j+1}^2] = \int_{\mathbb{R}} (t-\alpha_j)\tilde{\pi}_{j+1}(t)\,\frac{\partial\tilde{\pi}_j(t)}{\partial m_k}\,\mathrm{d}\lambda(t). \tag{2.1.86}$$

Now note from the three-term recurrence relation (2.1.84), with j replaced by $j+1$, that

$$(t-\alpha_j)\tilde\pi_{j+1}(t) = \sqrt{\beta_{j+2}}\,\tilde\pi_{j+2}(t) + (\alpha_{j+1}-\alpha_j)\tilde\pi_{j+1}(t) + \sqrt{\beta_{j+1}}\,\tilde\pi_j(t).$$

Inserting this into the right-hand side of (2.1.86) and using again orthonormality and (2.1.83) gives

$$\frac{\partial\sqrt{\beta_{j+1}}}{\partial m_k} - \tfrac{1}{2}\sqrt{\beta_{j+1}}c_k[\tilde\pi_{j+1}^2] = -\tfrac{1}{2}\sqrt{\beta_{j+1}}c_k[\tilde\pi_j^2],$$

that is,

$$\frac{\partial\sqrt{\beta_{j+1}}}{\partial m_k} = \tfrac{1}{2}\sqrt{\beta_{j+1}}c_k[\tilde\pi_{j+1}^2 - \tilde\pi_j^2],$$

or, multiplying by $2\sqrt{\beta_{j+1}}$,

$$\frac{\partial\beta_{j+1}}{\partial m_k} = c_k[\beta_{j+1}(\tilde\pi_{j+1}^2 - \tilde\pi_j^2)]. \tag{2.1.87}$$

This holds not only for $j \ge 0$, but also for $j=-1$, since $\beta_0 = \int_{\mathbb{R}} 1\cdot \mathrm{d}\lambda(t)$, hence, by Lemma 2.21,

$$\frac{\partial\beta_0}{\partial m_k} = c_k[1] = \beta_0 c_k[1/\beta_0] = \beta_0 c_k[\tilde\pi_0^2 - \tilde\pi_{-1}^2]$$

since $\tilde\pi_0^2 = 1/\beta_0$ and $\tilde\pi_{-1}^2 = 0$.

To isolate the derivative of α_j in (2.1.85), we multiply by $\tilde\pi_j$ and integrate. Similarly as above, but now using (2.1.82), one gets

$$-\sqrt{\beta_{j+1}}\,c_k[\tilde\pi_j\tilde\pi_{j+1}] = -\frac{\partial\alpha_j}{\partial m_k} + \int_{\mathbb{R}}(t-\alpha_j)\tilde\pi_j(t)\,\frac{\partial\tilde\pi_j(t)}{\partial m_k}\,\mathrm{d}\lambda(t),$$

and from (2.1.84) solved for $(t-\alpha_j)\tilde\pi_j(t)$, using again orthonormality,

$$-\sqrt{\beta_{j+1}}\,c_k[\tilde\pi_j\tilde\pi_{j+1}] = -\frac{\partial\alpha_j}{\partial m_k} - \sqrt{\beta_j}\,c_k[\tilde\pi_{j-1}\tilde\pi_j],$$

that is,

$$\frac{\partial\alpha_j}{\partial m_k} = c_k[\sqrt{\beta_{j+1}}\,\tilde\pi_j\tilde\pi_{j+1} - \sqrt{\beta_j}\,\tilde\pi_{j-1}\tilde\pi_j]. \tag{2.1.88}$$

Equations (2.1.88) and (2.1.87) (with j replaced by $j-1$) prove (2.1.79) in view of (2.1.80). □

Corollary 1 to Theorem 2.22 Let $\widetilde{\boldsymbol\Psi} \in \mathbb{R}^{2n\times 2n}$ be the matrix with elements $(\widetilde{\boldsymbol\Psi})_{\ell k} = c_k[\tilde\psi_\ell]$, $k=0,1,\dots,2n-1$; $\ell = 0,1,\dots,2n-1$. Then, the *absolute condition number* of $\boldsymbol{K}_n$ at the point $\boldsymbol{m}$, with the matrix norm being the infinity or Frobenius norm, is given by

$$(\operatorname{cond}\boldsymbol{K}_n)(\boldsymbol{m}) = \|\widetilde{\boldsymbol\Psi}\|. \tag{2.1.89}$$

Specifically,

$$\|\widetilde{\boldsymbol\Psi}\|_\infty = \max_{0\le\ell\le 2n-1}\sum_{k=0}^{2n-1}|c_k[\tilde\psi_\ell]|, \quad \|\widetilde{\boldsymbol\Psi}\|_F = \left(\sum_{\ell=0}^{2n-1}\sum_{k=0}^{2n-1}c_k^2[\tilde\psi_\ell]\right)^{1/2}. \tag{2.1.90}$$

Proof Matrix $\widetilde{\boldsymbol{\Psi}}$ differs from $\partial \boldsymbol{K}_n/\partial \boldsymbol{m}$ in (2.1.78) only in the ordering of the rows. Since neither the infinity nor the Frobenius norm depends on the ordering of rows, eqn (2.1.89) follows immediately from Definition 2.5 of the absolute condition number. Equation (2.1.90) follows trivially from (2.1.79). □

Corollary 2 to Theorem 2.22 The *relative condition number* of $\boldsymbol{K}_n$ in the sense of (2.1.17) and (2.1.18) is given by

$$(\operatorname{cond} \boldsymbol{K}_n)(\boldsymbol{m}) = \|\boldsymbol{C}(\boldsymbol{m})\|, \tag{2.1.91}$$

where

$$\boldsymbol{C}(\boldsymbol{m}) = [c_{jk}(\boldsymbol{m})]_{j,k=0}^{2n-1}$$

and

$$c_{jk}(\boldsymbol{m}) = \frac{m(m_k)|c_k[\tilde{\psi}_{2j+1}]|}{m(\alpha_j)}\,, \quad c_{j+n,k}(\boldsymbol{m}) = \frac{m(m_k)|c_k[\tilde{\psi}_{2j}]|}{m(\beta_j)}\,, \qquad j = 0, 1, \ldots, n-1. \tag{2.1.92}$$

Here, the polynomials $\tilde{\psi}_0, \tilde{\psi}_1, \ldots, \tilde{\psi}_{2n-1}$ are as defined in (2.1.80) and $m(\,\cdot\,)$ is the mollifier function (2.1.11).

Proof An immediate consequence of Theorem 2.22. □

Corollary 3 to Theorem 2.22 Let $\pi_k(\,\cdot\,) = \pi_k(\,\cdot\,; \mathrm{d}\lambda)$ denote the monic orthogonal polynomials with respect to the measure $\mathrm{d}\lambda$ (cf. Definition 1.3), and define

$$\begin{aligned} \psi_{2j}(t) &= \frac{1}{\beta_0\beta_1\cdots\beta_{j-1}}\left(\pi_j^2(t) - \beta_j\pi_{j-1}^2(t)\right), \\ \psi_{2j+1}(t) &= \frac{1}{\beta_0\beta_1\cdots\beta_j}\left(\pi_j(t)\pi_{j+1}(t) - \beta_j\pi_{j-1}\pi_j(t)\right), \\ &\qquad\qquad j = 0, 1, \ldots, n-1, \end{aligned} \tag{2.1.93}$$

where for $j = 0$ the empty product of the βs in the first relation is to be taken equal to 1. With $\boldsymbol{\Psi} \in \mathbb{R}^{2n\times 2n}$ defined by $(\boldsymbol{\Psi})_{\ell k} = c_k[\psi_\ell]$, there holds

$$(\operatorname{cond} \boldsymbol{K}_n)(\boldsymbol{m}) = \|\boldsymbol{\Psi}\|, \tag{2.1.94}$$

with the norm $\|\,\cdot\,\|$ as in Corollary 1.

Proof One easily checks, on the basis of (1.3.12), (1.3.7), and (2.1.80), that $\tilde{\psi}_{2j} = \psi_{2j}$ and $\tilde{\psi}_{2j+1} = \psi_{2j+1}$. □

It may be worth noting that the condition of $\boldsymbol{K}_n$ depends on the measure $\mathrm{d}\lambda$ entirely through the polynomials $\tilde{\psi}_k$ resp. ψ_k. The choice of the modified moments is reflected in the linear functionals c_k.

Example 2.23 *Chebyshev measure* on $[0,1]$ and *ordinary moments*.

As in Example 2.12, we take $\mathrm{d}\lambda(t) = [t(1-t)]^{-1/2}\,\mathrm{d}t$ and assume $\boldsymbol{m} = \boldsymbol{\mu}$, that is, $p_k(t) = t^k$, or $c_k[q] = q^{(k)}(0)/k!$ in (2.1.75). Well-known properties of Chebyshev polynomials can be used to show that (Fischer, 1996, pp. 229–230) $\tilde{\psi}_1 = \frac{1}{2}T_1^*$, $\tilde{\psi}_2 = \frac{1}{8}T_2^*$, and $\tilde{\psi}_{2j+1} = \frac{1}{4}(T_{2j+1}^* - T_{2j-1}^*)$, $\tilde{\psi}_{2j} = \frac{1}{16}(T_{2j}^* - T_{2j-2}^*)$, $j \geq 1$, where $T_k^*(t) = T_k(2t-1)$ are the "shifted" Chebyshev polynomials. It then follows from Corollary 1 to Theorem 2.22 that (Fischer, 1996, Theorem 2)

$$\left\| \frac{\partial \boldsymbol{K}_n}{\partial \boldsymbol{\mu}} \right\|_\infty = 4U_{2n-3}(3), \quad n \geq 2, \tag{2.1.95}$$

where U_{2n-3} is the Chebyshev polynomial of the second kind of degree $2n-3$ (cf. (1.5.5)). It is interesting to compare this with the lower bound for $(\operatorname{cond} \boldsymbol{G}_n)(\boldsymbol{\mu})$ in (2.1.43). Equation (2.1.95) gives

$$\left\| \frac{\partial \boldsymbol{K}_n}{\partial \boldsymbol{\mu}} \right\|_\infty = \frac{2(17-6\sqrt{8})}{\sqrt{8}}\,(17+6\sqrt{8})^n, \tag{2.1.96}$$

whereas (2.1.43) is

$$(\operatorname{cond} \boldsymbol{G}_n)(\boldsymbol{\mu}) > \frac{1}{48n^2}\,(17+6\sqrt{8})^n. \tag{2.1.97}$$

Thus, the exponential rate of growth is exactly the same in either case, although the coefficient in (2.1.97) naturally is smaller than in (2.1.96).

Example 2.24 *Chebyshev measure* on $[0,1]$ and *Bernstein polynomials*.

Choosing for p_k the Bernstein polynomials (cf. Example 2.9), one computes from (2.1.89) that (Fischer, 1996, Theorem 3)

$$(\operatorname{cond} \boldsymbol{K}_n)(\boldsymbol{\mu}) \sim \frac{1}{8}\sqrt{\frac{\pi n}{2}}\,4^n, \quad n \to \infty. \tag{2.1.98}$$

This still exhibits exponential growth, though at a considerably slower rate than in (2.1.96).

Example 2.25 *Chebyshev measure* on $[-1,1]$ and *Lagrange interpolation polynomials*.

Choosing for p_k Lagrange interpolation polynomials (cf. Example 2.10), one finds, rather surprisingly, that (Fischer, 1996, Theorem 5)

$$(\operatorname{cond} \boldsymbol{K}_n)(\boldsymbol{\mu}) \leq 2n, \tag{2.1.99}$$

independently of the choice of interpolation nodes (as long as they are distinct and contained in $[-1,1]$). Slow polynomial growth, as in (2.1.99), looks extremely attractive, but unfortunately no algorithm is presently known that would compute recursion coefficients from Lagrange modified moments. (The latter could be computed by Gaussian quadrature.)

2.1.7 *Modified Chebyshev algorithm*

For the choice of modified moments indicated in Example 2.8, which involves orthogonal polynomials $p_k(\,\cdot\,) = p_k(\,\cdot\,; \mathrm{d}\ell)$, we now develop an algorithm implementing the map $\boldsymbol{K}_n : \boldsymbol{m} \mapsto \boldsymbol{\rho}$. The algorithm is a generalization from ordinary to modified moments of an algorithm due to Chebyshev (1859, Oeuvres I, p. 482); in Gautschi (1982b, §2.4) we, therefore, called it the *modified Chebyshev algorithm*. It actually can be applied with any system of monic polynomials $\{p_k\}$ that satisfies a three-term recurrence relation

$$\begin{aligned} p_{k+1}(t) &= (t - a_k)p_k(t) - b_k p_{k-1}(t), \quad k = 0, 1, 2, \ldots, \\ p_{-1}(t) &= 0, \quad p_0(t) = 1 \end{aligned} \tag{2.1.100}$$

with $a_k \in \mathbb{R}$ and $b_k \geq 0$. In the case $a_k = b_k = 0$, it reduces to Chebyshev's original algorithm.

We introduce the "mixed moments"

$$\sigma_{k\ell} = \int_{\mathbb{R}} \pi_k(t) p_\ell(t)\, \mathrm{d}\lambda(t), \quad k, \ell \geq -1, \tag{2.1.101}$$

where $\pi_k(\,\cdot\,) = \pi_k(\,\cdot\,; \mathrm{d}\lambda)$ are the monic orthogonal polynomials with respect to the given measure $\mathrm{d}\lambda$ (cf. Theorem 1.27). By orthogonality, one has $\sigma_{k\ell} = 0$ for $k > \ell$, and since $tp_{k-1}(t) = \pi_k(t) + \cdots$, where dots stand for a polynomial of degree $< k$, there holds

$$\int_{\mathbb{R}} \pi_k^2(t)\, \mathrm{d}\lambda(t) = \int_{\mathbb{R}} \pi_k(t) t p_{k-1}(t)\, \mathrm{d}\lambda(t) = \sigma_{kk}, \quad k \geq 1.$$

The relation $\sigma_{k+1,k-1} = 0$, together with the three-term recurrence relation for π_k (see (1.3.2)),

$$\begin{aligned} \pi_{k+1}(t) &= (t - \alpha_k)\pi_k(t) - \beta_k \pi_{k-1}(t), \quad k = 0, 1, 2, \ldots, \\ \pi_{-1}(t) &= 0, \quad \pi_0(t) = 1, \end{aligned} \tag{2.1.102}$$

thus yields, again using orthogonality,

$$0 = \int_{\mathbb{R}} [(t - \alpha_k)\pi_k(t) - \beta_k \pi_{k-1}(t)] p_{k-1}(t)\, \mathrm{d}\lambda(t) = \sigma_{kk} - \beta_k \sigma_{k-1,k-1},$$

that is,

$$\beta_k = \frac{\sigma_{kk}}{\sigma_{k-1,k-1}}, \quad k = 1, 2, 3, \ldots. \tag{2.1.103}$$

(Recall that $\beta_0 = \int_{\mathbb{R}} \mathrm{d}\lambda(t) = m_0$.) Similarly, $\sigma_{k+1,k} = 0$ gives

$$\begin{aligned} 0 &= \int_{\mathbb{R}} [(t - \alpha_k)\pi_k(t) - \beta_k \pi_{k-1}(t)] p_k(t)\, \mathrm{d}\lambda(t) \\ &= \int_{\mathbb{R}} \pi_k(t) t p_k(t)\, \mathrm{d}\lambda(t) - \alpha_k \sigma_{kk} - \beta_k \sigma_{k-1,k}. \end{aligned}$$

Using (2.1.100) in the form

$$tp_k(t) = p_{k+1}(t) + a_k p_k(t) + b_k p_{k-1}(t) \tag{2.1.104}$$

then yields

$$0 = \sigma_{k,k+1} + (a_k - \alpha_k)\sigma_{kk} - \beta_k \sigma_{k-1,k},$$

hence, together with (2.1.103) and the fact that $\sigma_{-1,\ell} = 0$,

$$\begin{aligned} \alpha_0 &= a_0 + \frac{\sigma_{01}}{\sigma_{00}}, \\ \alpha_k &= a_k - \frac{\sigma_{k-1,k}}{\sigma_{k-1,k-1}} + \frac{\sigma_{k,k+1}}{\sigma_{kk}}, \quad k = 1, 2, 3, \ldots . \end{aligned}$$

The σs, in turn, satisfy the recursion

$$\sigma_{k\ell} = \sigma_{k-1,\ell+1} - (\alpha_{k-1} - a_\ell)\sigma_{k-1,\ell} - \beta_{k-1}\sigma_{k-2,\ell} + b_\ell \sigma_{k-1,\ell-1},$$

as follows from (2.1.102) (with k replaced by $k-1$) and (2.1.104) (with k replaced by ℓ). Thus, to compute the first n recursion coefficients from the first $2n$ modified moments, one has the following algorithm.

Algorithm 2.1 (Modified Chebyshev algorithm)

Initialization:

$$\begin{aligned} &\alpha_0 = a_0 + \frac{m_1}{m_0}, \\ &\beta_0 = m_0, \\ &\sigma_{-1,\ell} = 0, \quad \ell = 1, 2, \ldots, 2n-2, \\ &\sigma_{0,\ell} = m_\ell, \quad \ell = 0, 1, \ldots, 2n-1. \end{aligned} \tag{2.1.105}$$

Continuation (if $n > 1$): for $k = 1, 2, \ldots, n-1$ do

$$\begin{aligned} \sigma_{k\ell} &= \sigma_{k-1,\ell+1} - (\alpha_{k-1} - a_\ell)\sigma_{k-1,\ell} - \beta_{k-1}\sigma_{k-2,\ell} \\ &\quad + b_\ell \sigma_{k-1,\ell-1}, \quad \ell = k, k+1, \ldots, 2n-k-1, \\ \alpha_k &= a_k + \frac{\sigma_{k,k+1}}{\sigma_{kk}} - \frac{\sigma_{k-1,k}}{\sigma_{k-1,\ell-1}}, \\ \beta_k &= \frac{\sigma_{kk}}{\sigma_{k-1,k-1}}. \end{aligned} \tag{2.1.106}$$

The algorithm requires as input $\{m_\ell\}_{\ell=0}^{2n-1}$ and $\{a_k, b_k\}_{k=0}^{2n-2}$, and produces $\{\alpha_k, \beta_k\}_{k=0}^{n-1}$. The complexity in terms of arithmetic operations is $O(n^2)$.

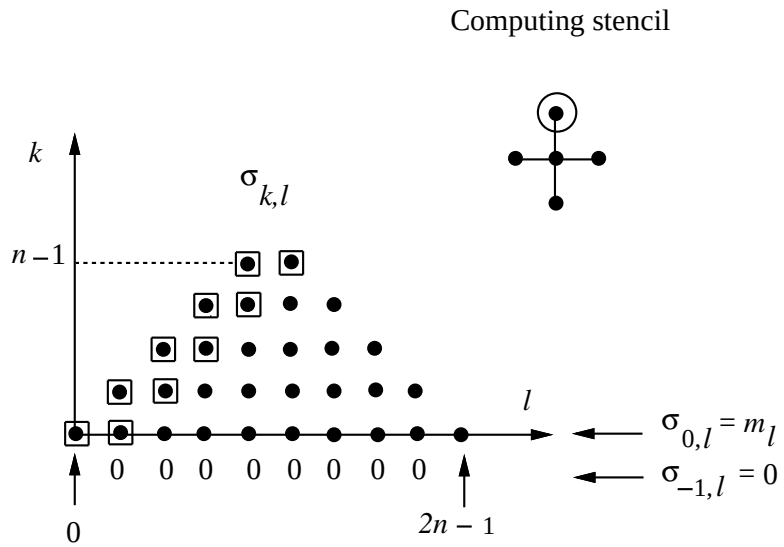

FIG. 2.1. The modified Chebyshev algorithm, schematically.

The algorithm is summarized schematically in Fig. 2.1. The computing stencil indicates the location of the five entries in the σ-tableau that are involved in relation (2.1.106). The circled entry in the stencil is the one the algorithm computes in terms of the other four. The entries in boxes are those used to compute α_k and β_k. The `OPQ` routine `chebyshev.m` implements the algorithm.

The success of Algorithm 2.1 depends on the ability to compute all required modified moments m_ℓ accurately and reliably. Most frequently, these moments are obtained from recurrence relations, judiciously employed, as, for example, in the case of Chebyshev or Gegenbauer moments (Piessens and Branders (1973), Lewanowicz (1979), (1994a)). Sometimes they can be computed directly in terms of special functions, or in integer form (Gautschi (1970, Examples (ii) and (iii)), Wheeler and Blumstein (1972), Blue (1979), Gautschi (1979), Gatteschi (1980)).

Another possibility is to run Algorithm 2.1 with approximate modified moments obtained by discretizing the integral defining them; see §2.2.6.

2.1.8 *Finite expansions in orthogonal polynomials*

Mixed moments and the recurrence relation for them have other applications; for example, to convert a finite expansion of a polynomial in terms of orthogonal polynomials into one in terms of another set of orthogonal polynomials. Before discussing this, we develop an efficient algorithm for evaluating certain finite expansions.

2.1.8.1 *Clenshaw's algorithm* Let $y_k = y_k(t)$ be functions satisfying a three-term recurrence relation

$$y_{k+1} = (t - \alpha_k)y_k - \beta_k y_{k-1}, \quad k = 0, 1, 2, \ldots, \tag{2.1.107}$$

with given initial values y_0 and y_{-1}. We are interested in finite sums

$$r(t) = \sum_{j=0}^{n} c_j y_j(t). \tag{2.1.108}$$

The following algorithm is an efficient way to evaluate them.

Algorithm 2.2 (Clenshaw's algorithm)

Initialization:

$$u_n = c_n, \quad u_{n+1} = 0. \tag{2.1.109}$$

Continuation (if $n > 0$): for $k = n-1, n-2, \ldots, 0$ do

$$u_k = (t - \alpha_k)u_{k+1} - \beta_{k+1}u_{k+2} + c_k. \tag{2.1.110}$$

Result:

$$r(t) = u_0 y_0 - \beta_0 u_1 y_{-1}. \tag{2.1.111}$$

The validity of Algorithm 2.2 is best seen by writing (2.1.107) in matrix form as

$$\boldsymbol{L}\boldsymbol{y}(t) = \boldsymbol{\rho}, \quad \boldsymbol{\rho} = [y_0, -\beta_0 y_{-1}, 0, \ldots, 0]^{\mathrm{T}} \in \mathbb{R}^{n+1},$$

where

$$\boldsymbol{L} = \begin{bmatrix} 1 & & & \boldsymbol{0} \\ \alpha_0 - t & 1 & & \\ \beta_1 & \alpha_1 - t & 1 & \\ & \ddots & \ddots & \ddots \\ \boldsymbol{0}^{\mathrm{T}} & \beta_{n-1} & \alpha_{n-1} - t & 1 \end{bmatrix}, \quad \boldsymbol{y}(t) = \begin{bmatrix} y_0(t) \\ y_1(t) \\ y_2(t) \\ \vdots \\ y_n(t) \end{bmatrix}.$$

The recurrence relation in Algorithm 2.2 is then simply $\boldsymbol{L}^{\mathrm{T}}\boldsymbol{u} = \boldsymbol{c}$, where $\boldsymbol{u}^{\mathrm{T}} = [u_0, u_1, \ldots, u_n]$, $\boldsymbol{c}^{\mathrm{T}} = [c_0, c_1, \ldots, c_n]$. Thus,

$$r(t) = \boldsymbol{c}^{\mathrm{T}}\boldsymbol{y}(t) = \boldsymbol{c}^{\mathrm{T}}\boldsymbol{L}^{-1}\boldsymbol{\rho} = ((\boldsymbol{L}^{\mathrm{T}})^{-1}\boldsymbol{c})^{\mathrm{T}}\boldsymbol{\rho} = \boldsymbol{u}^{\mathrm{T}}\boldsymbol{\rho},$$

proving (2.1.111).

Algorithm 2.2 is implemented in the `OPQ` routine `clenshaw.m`.

In the case $y_k = \pi_k$ of monic orthogonal polynomials, one has $y_0 = 1$, $y_{-1} = 0$, so that $r(t) = u_0$. For the important special case of a Chebyshev expansion,

$$s(t) = \tfrac{1}{2}d_0 + \sum_{j=1}^{n} d_j T_j(t), \tag{2.1.112}$$

Algorithm 2.2 can be given the following form.

Algorithm 2.3 (Clenshaw's algorithm for a Chebyshev expansion)
Initialization:

$$v_n = d_n, \quad v_{n+1} = 0, \quad v_{n+2} = 0. \tag{2.1.113}$$

Continuation (if $n > 0$): for $k = n-1, n-2, \ldots, 0$ do

$$v_k = 2tv_{k+1} - v_{k+2} + d_k. \tag{2.1.114}$$

Result:

$$s(t) = \tfrac{1}{2}(v_0 - v_2). \tag{2.1.115}$$

(The last relation in (2.1.113) seems redundant, but is included to make the algorithm work also for $n = 0$.) To verify Algorithm 2.3, one must first write (2.1.112) in terms of the monic Chebyshev polynomials, $T_j^0(t) = T_j(t)/2^{j-1}$ $(j \geq 1)$, $T_0^0(t) = T_0(t)$, so that $c_0 = \frac{1}{2}d_0$, $c_j = 2^{j-1}d_j$ $(j \geq 1)$. Moreover, the recursion coefficients are $\alpha_k = 0$, $\beta_1 = \frac{1}{2}$, $\beta_k = \frac{1}{4}$ $(k \geq 2)$; cf. Table 1.1. Algorithm 2.2 then becomes

$$\begin{aligned} u_n &= 2^{n-1}d_n, \quad u_{n+1} = 0, \\ u_k &= tu_{k+1} - \tfrac{1}{4}u_{k+2} + 2^{k-1}d_k, \\ &\qquad k = n-1, n-2, \ldots, 1, \\ u_0 &= tu_1 - \tfrac{1}{2}u_2 + \tfrac{1}{2}d_0. \end{aligned}$$

Letting $v_k = u_k/2^{k-1}$ $(k \geq 1)$, $v_0 = u_0$ yields Algorithm 2.3 except for the last step of the recursion, which should be $v_0 = tv_1 - v_2 + d_0/2$, but instead defines $v_0^* = 2tv_1 - v_2 + d_0$. To compensate for this, one writes

$$\begin{aligned} v_0 &= tv_1 - v_2 + \tfrac{1}{2}d_0 = tv_1 + v_0^* - 2tv_1 - d_0 + \tfrac{1}{2}d_0 \\ &= -tv_1 - \tfrac{1}{2}d_0 + v_0^* = -v_0 - v_2 + \tfrac{1}{2}d_0 - \tfrac{1}{2}d_0 + v_0^* \\ &= -v_0 - v_2 + v_0^*, \end{aligned}$$

that is, $2v_0 = v_0^* - v_2$, and hence the result (2.1.115) for $s(t) = v_0$.

Algorithm 2.3 is implemented in the `OPQ` routine `clenshaw_cheb.m`

2.1.8.2 *Conversion algorithm* Let $\{p_\ell\}$ be the monic orthogonal polynomials of §2.1.7 satisfying the three-term recurrence relation (2.1.100) with coefficients $a_k \in \mathbb{R}$ and $b_k \geq 0$ and orthogonal with respect to a measure $\mathrm{d}\ell$ if $b_k > 0$. Consider

$$p(t) = \sum_{\ell=0}^{n} c_\ell p_\ell(t). \tag{2.1.116}$$

Let $\{\pi_k\}$ as in §2.1.8.1 be another set of monic polynomials, orthogonal with respect to the measure $\mathrm{d}\lambda$, satisfying the three-term recurrence relation (2.1.102)

with coefficients α_k and β_k. The problem is to find the expansion of p in terms of the π_k,

$$p(t) = \sum_{k=0}^{n} \gamma_k \pi_k(t), \tag{2.1.117}$$

knowing the expansion (2.1.116). An algorithm that computes the coefficients γ_k from the known coefficients c_ℓ is called a *conversion algorithm*.

We start by expressing p_ℓ in terms of the π_k,

$$p_\ell(t) = \sum_{k=0}^{\ell} d_{\ell k} \pi_k(t). \tag{2.1.118}$$

By orthogonality of π_k,

$$(p_\ell, \pi_k)_{\mathrm{d}\lambda} = d_{\ell k}(\pi_k, \pi_k)_{\mathrm{d}\lambda} = d_{\ell k}(p_k, \pi_k)_{\mathrm{d}\lambda},$$

or, by the symmetry of the inner product,

$$d_{\ell k} = \frac{\sigma_{k\ell}}{\sigma_{kk}}, \quad k = 0, 1, \ldots, \ell, \tag{2.1.119}$$

where $\sigma_{k\ell}$ are the mixed moments of (2.1.101). Inserting (2.1.118) and (2.1.119) in (2.1.116) yields

$$p(t) = \sum_{\ell=0}^{n} c_\ell p_\ell(t) = \sum_{\ell=0}^{n} c_\ell \sum_{k=0}^{\ell} \frac{\sigma_{k\ell}}{\sigma_{kk}} \pi_k(t) = \sum_{k=0}^{n} \left(\frac{1}{\sigma_{kk}} \sum_{\ell=k}^{n} \sigma_{k\ell} c_\ell \right) \pi_k(t),$$

that is,

$$\gamma_k = \frac{1}{\sigma_{kk}} \sum_{\ell=k}^{n} \sigma_{k\ell} c_\ell, \quad k = 0, 1, \ldots, n.$$

Since $\sigma_{00} = \beta_0$, $\sigma_{-1,\ell} = \sigma_{k,-1} = 0$, and $\sigma_{k\ell} = 0$ for $k > \ell$, we can compute $\sigma_{k\ell}$, $k = 0, 1, \ldots, n$; $\ell = k, k+1, \ldots, n$ by the scheme indicated in Fig. 2.1, but solving for the East entry in the computing stencil rather than for the North entry. Thus, one computes $\sigma_{k\ell}$ in the order σ_{01}, σ_{11}; $\sigma_{02}, \sigma_{12}, \sigma_{22}$; $\ldots$; $\sigma_{0n}, \sigma_{1n}, \ldots, \sigma_{nn}$; using the recursion in (2.1.106). This gives rise to the following algorithm.

Algorithm 2.4 (Conversion algorithm)

Initialization:

$$\begin{aligned} &\sigma_{00} = \beta_0, \\ &\sigma_{-1,\ell} = 0, \quad \ell = 0, 1, \ldots, n, \\ &\sigma_{k,k-1} = \sigma_{k+1,k-1} = 0, \quad k = 0, 1, \ldots, n. \end{aligned} \tag{2.1.120}$$

Continuation (if $n > 0$): for $\ell = 0, 1, \ldots, n-1$ do

$$\sigma_{k,\ell+1} = \sigma_{k+1,\ell} + (\alpha_k - a_\ell)\sigma_{k\ell} + \beta_k\sigma_{k-1,\ell} - b_\ell\sigma_{k,\ell-1}, \quad k = 0, 1, \ldots, \ell+1. \tag{2.1.121}$$

Conversion:

$$\gamma_k = \frac{1}{\sigma_{kk}} \sum_{\ell=k}^{n} \sigma_{k\ell} c_\ell, \quad k = 0, 1, \ldots, n. \tag{2.1.122}$$

The algorithm is implemented in the `OPQ` routine `convert.m`.

2.1.9 *Examples*

Our interest, as in Examples 2.14–2.16, is again to compare theory with practice, that is, to see how condition numbers correlate with actual error growth. The precise meaning of the latter is described in the paragraph preceding Example 2.14.

We begin with a measure of discrete type for which Chebyshev originally, in connection with discrete least squares approximation (cf. §3.2), developed his algorithm.

Example 2.26 $\mathrm{d}\lambda_N(t) = (1/N)\sum_{k=0}^{N-1} \delta(x - k/N)\,\mathrm{d}t$.

The monic orthogonal polynomials $\pi_k(\,\cdot\,) = \pi_k(\,\cdot\,; \mathrm{d}\lambda_N)$ are the discrete Chebyshev polynomials transformed to the interval $[0, 1)$. Although the recursion coefficients are known explicitly (cf. Commentary to Table 1.2 regarding discrete Chebyshev polynomials), it is instructive to examine the condition of the map $\boldsymbol{G}_n$, both in the case of ordinary moments

$$\mu_r = \int_0^1 t^r \,\mathrm{d}\lambda_N(t) = \frac{1}{N} \sum_{k=0}^{N-1} \left(\frac{k}{N}\right)^r, \quad r = 0, 1, \ldots, 2n-1 \tag{2.1.123}$$

(the case considered by Chebyshev), and modified moments; for example, those relative to monic shifted Legendre polynomials P_r^{*0} (cf. Table 1.1),

$$m_r = \int_0^1 P_r^{*0}(t) \,\mathrm{d}\lambda_N(t) = \frac{1}{N} \sum_{k=0}^{N-1} P_r^{*0}\left(\frac{k}{N}\right), \quad r = 0, 1, \ldots, 2n-1, \tag{2.1.124}$$

where $n \le N - 1$. In the former case, we compute the lower bound of Theorem 2.11 for $(\operatorname{cond} \boldsymbol{G}_n)(\boldsymbol{\mu})$, in the latter case the integral expression in Theorem 2.17 for $(\operatorname{cond} \widetilde{\boldsymbol{G}}_n)(\widetilde{\boldsymbol{m}})$. Both are appropriate since all moments and recursion coefficients are less than 1 in modulus. The Gaussian nodes τ_ν and weights λ_ν needed for this computation are generated by the methods of §3.1.1 using the known recursion coefficients of $\mathrm{d}\lambda_N$.

Table 2.4 *Condition number and error magnification for discrete 20-point Chebyshev measure on* $[0,1)$ *using ordinary moments.*

n	(2.1.36)	mag α	mag β
2	1.11(1)	2.25(0)	1.25(–1)
5	1.24(5)	4.34(4)	2.32(3)
8	2.50(9)	7.71(8)	3.40(7)
11	1.00(14)	2.60(13)	1.01(12)

Table 2.4, computed with the `OPQ` routine `Table2_4.m`, illustrates (once again!) the ill-conditioning of the map $\boldsymbol{G}_n(\boldsymbol{\mu})$. Here, $N = 20$ and $n = 2, 5, 8, 11$, and accuracy is seen to be lost at a rate somewhat faster than one decimal digit per degree!

More stable, though not entirely unproblematic, is the modified Chebyshev algorithm using the Legendre moments (2.1.124). This is shown in Table 2.5, computed with the `OPQ` routine `Table2_5.m`, for $N = 10, 20, 40, 80$ and selected values of n. It is seen that as n approaches N, the condition of $\widetilde{\boldsymbol{G}}_n(\widetilde{\boldsymbol{m}})$, and with

Table 2.5 *Condition number and error magnification for discrete N-point Chebyshev measure on* $[0,1)$ *using Legendre moments.*

N	n	(2.1.50)	mag α	mag β	N	n	(2.1.50)	mag α	mag β
10	5	2.47(0)	5.00(–1)	6.25(–2)	40	15	3.71(1)	6.75(0)	2.00(0)
	10	5.01(4)	4.05(3)	1.22(2)		25	2.34(6)	4.67(5)	4.65(4)
20	5	1.01(0)	2.50(–1)	6.25(–2)		35	8.22(14)	1.10(14)	3.97(12)
	10	2.50(1)	9.00(0)	1.22(0)	80	10	9.26(–1)	2.50(–1)	6.25(–2)
	15	3.67(4)	1.90(4)	1.37(3)		20	1.56(1)	4.00(0)	7.19(–1)
	20	3.72(10)	1.65(10)	2.00(8)		30	1.04(4)	1.89(3)	3.10(2)
40	5	8.90(–1)	2.50(–1)	2.00(0)		40	1.29(8)	1.03(7)	1.43(6)
	10	1.73(0)	5.00(–1)	2.00(0)		50	4.45(13)	2.00(12)	1.62(11)

it the error magnification, grows very significantly. The reason for this lies in the distribution of the Gauss nodes τ_ν for $\mathrm{d}\lambda_N$, which, though apparently all weak in the sense described before Theorem 2.19, become more equally spaced as n approaches N. (They *are* equally spaced for $n = N$.) The Hermite interpolation polynomials h_ν and k_ν in (2.1.51), therefore, begin to exhibit the violent oscillations characteristic of equally spaced points, which lead to large peaks of g_n between the first few, and last few, Gaussian nodes τ_ν and to large maxima at the end points of $[0,1]$. Related to this is an instability phenomenon associated with the three-term reccurence relation; cf. §2.2.3.1.

The next two examples illustrate cases of almost perfect stability.

Example 2.27 $\mathrm{d}\lambda(t) = t^\alpha \ln(1/t)\,\mathrm{d}t$ on $[0,1]$, $\alpha > -1$.

Here, the modified moments m_r with respect to the monic shifted Legendre polynomials $p_k(t) = (k!^2/(2k)!)P_k(2t-1)$ can be obtained in closed form; cf. Gautschi (1979). If α is not an integer, for example, one finds

$$\frac{(2r)!}{r!^2}\,m_r = \frac{1}{\alpha+1}\left\{\frac{1}{\alpha+1} + \sum_{\rho=1}^{r}\left(\frac{1}{\alpha+1+\rho} - \frac{1}{\alpha+1-\rho}\right)\right\}\prod_{\rho=1}^{r}\frac{\alpha+1-\rho}{\alpha+1+\rho}, \quad r = 0,1,2,\ldots. \tag{2.1.125}$$

(Similar formulae hold for integral α; see Blue (1979) for $\alpha = 0$ and Gautschi (1979) for $\alpha > 0$. Modified moments relative to shifted Jacobi polynomials of the more general measure $t^\alpha(1-t)^\beta \ln(1/t)\,\mathrm{d}t$, $\alpha > -1$, $\beta > -1$, are computed explicitly in Gatteschi (1980).) The modified Chebyshev algorithm for this example is implemented in the OPQ routine `r_jaclog.m`. Using it for $\alpha = -\frac{1}{2}, 0, \frac{1}{2}$ yields the results in Table 2.6, displayed in a format similar to the one adopted in Table 2.5. The errors are computed by comparison with quadruple-precision results

Table 2.6 *Condition number and error magnification for the measure in Example 2.27 using Legendre moments.*

α	n	(2.1.50)	mag α	mag β
$-\frac{1}{2}$	25	5.35(1)	1.65(1)	4.12(0)
	50	1.49(2)	3.72(1)	9.38(0)
	75	2.72(2)	3.72(1)	9.38(0)
	100	4.18(2)	3.72(1)	9.38(0)
0	25	5.39(1)	5.00(–1)	9.38(–2)
	50	1.50(2)	7.50(–1)	2.50(–1)
	75	2.73(2)	1.50(0)	3.75(–1)
	100	4.19(2)	1.50(0)	3.75(–1)
$\frac{1}{2}$	25	5.46(1)	7.50(–1)	1.25(–1)
	50	1.51(2)	7.50(–1)	1.25(–1)
	75	2.74(2)	1.25(0)	2.81(–1)
	100	4.21(2)	1.50(0)	3.44(–1)

obtained by the ORTHPOLq routine `qtest2.m`. For the details of the computations, see the OPQ routine `Table2_6.m`. The first 100 recurrence coefficients for the three values of α are available to 25 decimal places in the OPQ file `abjaclog`.

The condition of $\widetilde{\boldsymbol{G}}_n(\widetilde{\boldsymbol{m}})$ is seen to remain relatively small, even for values of n as large as 100, and the error magnification even smaller. The gradual (but slow) increase of $(\mathrm{cond}\,\widetilde{\boldsymbol{G}}_n)(\widetilde{\boldsymbol{m}})$ can be ascribed to a phenomenon similar to the one observed in Example 2.26, except that this time not all nodes τ_ν are weak, but only about the first two-thirds of them (when ordered increasingly). All remaining nodes appear to be strong, giving rise to the development of peaks and final upward surges of g_n as in Example 2.26. The height of the peaks,

nevertheless, is much lower here than before.

Some of the entries in the columns headed $\operatorname{mag}\alpha$ and $\operatorname{mag}\beta$ are seen to be identical for different values of n. This is because the maximum error magnification in α_k or β_k may be attained at the same value of k for different values of n.

Example 2.28 $\mathrm{d}\lambda(t) = t^\alpha[\ln(1/t)]^2\,\mathrm{d}t$ on $[-1,1]$, $\alpha > -1$.

With p_k again the monic shifted Legendre polynomials, the modified moments can be obtained from those of Example 2.27 by differentiation with respect to α and changing the sign. The result is

$$\frac{(2r)!}{r!^2}\,m_r = \frac{2}{(\alpha+1)^3}\left\{1 - 2(\alpha+1)\Sigma_1 + 2(\alpha+1)^2\Sigma_1^2 - 2(\alpha+1)^3\Sigma_2\right\}\Pi,$$

where

$$\Sigma_1 = \sum_{\rho=1}^{r} \frac{\rho}{(\rho+\alpha+1)(\alpha+1-\rho)}\,,$$

$$\Sigma_2 = \sum_{\rho=1}^{r} \frac{\rho}{(\rho+\alpha+1)^2(\alpha+1-\rho)^2}\,,$$

$$\Pi = \prod_{\rho=1}^{r} \frac{\alpha+1-\rho}{\alpha+1+\rho}\,.$$

Example 2.29 $\mathrm{d}\lambda(t) = w(t)\,\mathrm{d}t$ on $[-1,1]$ with $w(t) = [(1-k^2t^2)(1-t^2)]^{-1/2}$, $0 < k < 1$.

This is an example already considered by Christoffel (1877, Example 6) and much later by Rees (1945). What intrigued Christoffel was the fact that the orthogonal polynomials $\pi_r(\,\cdot\,) = \pi_r(\,\cdot\,;\mathrm{d}\lambda)$, when considered as functions of $x = \int_0^t w(t)\,\mathrm{d}t$, constitute a sequence of doubly periodic functions orthogonal in the sense

$$\int_{-K}^{K} \pi_r(t)\pi_s(t)\,\mathrm{d}x = 0, \quad r \neq s,$$

where K denotes the complete elliptic integral $K = \int_0^1 w(t)\,\mathrm{d}t$. Rees called the polynomials π_r *elliptic orthogonal polynomials* and the measure may be called *elliptic Chebyshev*.

Since $(1-k^2t^2)^{1/2}$ is analytic in a neighborhood of $[-1,1]$, the elliptic orthogonal polynomials must be "close" to the Chebyshev polynomials of the first kind and the associated Gaussian nodes τ_ν close to Chebyshev points. As a matter of fact, numerical evidence suggests that for all $0 < k < 1$, and all n, the Gauss nodes $\tau_\nu = \tau_\nu^{(n)}(\mathrm{d}\lambda)$ are all weak nodes and, moreover, the polynomial $g_n(\,\cdot\,;\mathrm{d}\lambda)$ never exceeds 1 on $[-1,1]$ (cf. Examples 2.18 and 2.20). This has been verified for values of n as large as 80, and values of k as close to 1 as $k^2 = 0.999$. It appears, therefore, that the absolute condition of $\widetilde{\boldsymbol{G}}_n(\widetilde{\boldsymbol{m}})$ is uniformly bounded, irrespective of the choice of modified moments. For the latter, it seems natural to

take those relative to the monic Chebyshev polynomials $p_0 = T_0$, $p_k = 2^{1-k}T_k$, $k = 1, 2, \ldots$. The modified Chebyshev algorithm then is found to work extremely well, producing results essentially accurate to machine precision for all values of n and k referred to above. (The errors were determined by comparison with quadruple-precision results obtained by the (simplified) `ORTHPOLq` routine `qtest1`.) For numerical illustrations, see the `OPQ` routine `Example2_29.m`, which uses the routine `r_elliptic.m` that implements the modified Chebyshev algorithm for this example.

The computation of the modified moments

$$m_r = \int_{-1}^{1} p_r(t)\,\mathrm{d}\lambda(t), \quad r = 0, 1, 2, \ldots, \tag{2.1.126}$$

however, is not entirely trivial. A procedure that has been utilized in Gautschi (1982b, Example 4.4) is the following. Let $t = \cos\theta$ in (2.1.126) to write

$$m_0 = \int_0^{\pi} \frac{\mathrm{d}\theta}{(1 - k^2\cos^2\theta)^{1/2}}, \quad m_r = \frac{1}{2^{r-1}} \int_0^{\pi} \frac{\cos r\theta}{(1 - k^2\cos^2\theta)^{1/2}}\,\mathrm{d}\theta. \tag{2.1.127}$$

Then, put $\varphi = \pi/2 - \theta$ in the Fourier expansion

$$\frac{1}{(1 - k^2\sin^2\varphi)^{1/2}} = C_0(k^2) + 2\sum_{n=1}^{\infty} C_n(k^2)\cos 2n\varphi$$

and substitute the result in (2.1.127). By virtue of the orthogonality of the cosine functions, one obtains

$$\begin{aligned} m_0 &= \pi C_0(k^2), \\ m_{2r} &= (-1)^r \frac{\pi}{2^{2r-1}} C_r(k^2), \quad r = 1, 2, 3, \ldots, \end{aligned} \tag{2.1.128}$$

while, of course, $m_{2r-1} = 0$, $r = 1, 2, 3, \ldots$. On the other hand, $y_n = C_n(k^2)$, $n = 0, 1, 2, \ldots$, is a minimal solution in the sense of Definition 1.42 of the three-term recurrence relation

$$(n + \tfrac{1}{2})y_{n+1} + n\,\frac{1 + q^2}{q}\,y_n + (n - \tfrac{1}{2})y_{n-1} = 0, \quad n = 1, 2, 3, \ldots, \tag{2.1.129}$$

where

$$q = \frac{k^2}{2 - k^2 + 2(1 - k^2)^{1/2}}, \tag{2.1.130}$$

and it satisfies

$$y_0 + 2\sum_{n=1}^{\infty} y_n = 1 \tag{2.1.131}$$

(see Luke (1969, p. 36)). Our continued fraction algorithm in Gautschi (1967a, eqn (3.9)), in conjunction with the normalizing condition (2.1.131), then yields

the Fourier coefficients $C_n(k^2)$, hence the modified moments in (2.1.128), very accurately and efficiently. The algorithm works well even when k^2 is quite close to 1. Note, in fact, that (2.1.129) is a difference equation of Poincaré type, with characteristic equation

$$u^2 + \frac{1+q^2}{q}\, u + 1 = 0, \quad 0 < q < 1,$$

having two real roots u_1 and u_2 with $|u_1| > 1 > |u_2|$ and

$$\left|\frac{u_1}{u_2}\right| = \frac{1}{q^2}\,.$$

(The minimal solution $y_n = C_n(k^2)$ "corresponds" to u_2.) If $k^2 = 1-\varepsilon$, $0 < \varepsilon < 1$, then by (2.1.130),

$$\frac{1}{q^2} = \left(\frac{1+\sqrt{\varepsilon}}{1-\sqrt{\varepsilon}}\right)^2 = 1 + 4\sqrt{\varepsilon} + 8\varepsilon + 12\varepsilon\sqrt{\varepsilon} + 16\varepsilon^2 + o(\varepsilon^2), \quad \varepsilon \to 0,$$

so that, when $k^2 = 0.999$, for example, one has $\varepsilon = 10^{-3}$, hence $|u_1/u_2| \approx 1.13$, which is still an adequate separation of the roots for the minimality of the solution y_n to take hold. The algorithm is implemented in the `OPQ` routine `mm_ell.m`.

Example 2.30 A measure of interest in the *diatomic linear chain* model (Wheeler, 1984) (cf. also Example 1.12).

This is the measure

$$\mathrm{d}\lambda(t) = \begin{cases} \frac{1}{\pi}|t-\frac{1}{2}|\{t(1-t)(t-\frac{1}{3})(t-\frac{2}{3})\}^{-1/2}\,\mathrm{d}t, & t \in [0,\frac{1}{3}] \cup [\frac{2}{3},1], \\ 0 & \text{otherwise}, \end{cases} \tag{2.1.132}$$

supported on two separate intervals, $[0, \frac{1}{3}]$ and $[\frac{2}{3}, 1]$, at each end point of which there is a "singularity of Chebyshev type." Although the recursion coefficients $\alpha_k(\mathrm{d}\lambda)$ and $\beta_k(\mathrm{d}\lambda)$ can be computed in closed form (cf. Gautschi (1984b)), the example is interesting since it provides a case for illustrating the proper choice of modified moments.

One could be tempted, and in fact it was tried in Wheeler (1984), to take modified moments based on the shifted Chebyshev polynomials, that is, to take $\mathrm{d}\ell(t) = \pi^{-1}[t(1-t)]^{-1/2}\,\mathrm{d}t$ on $[0,1]$. (For the accurate calculation of these modified moments, we refer to the cited article.) This, however, leads to serious instabilities. The reason is the particular pattern in which the Gaussian nodes $\tau_\nu = \tau_\nu(\mathrm{d}\lambda)$ are distributed. In view of Theorem 1.21, they are necessarily constrained to stay in the two support intervals except when n is odd, in which case one node is at the midpoint $t = \frac{1}{2}$. As a consequence, the polynomial $g_n(\,\cdot\,;\mathrm{d}\lambda)$ wiggles rapidly on these two intervals, remaining ≤ 1 there, but shoots up to a huge peak (double peak, if n is odd) on the central interval $[\frac{1}{3}, \frac{2}{3}]$. When $n = 40$,

for example, the peak value is of the order 10^{20}. Since the support of the chosen $\mathrm{d}\ell$ is the *whole* interval $[0,1]$, the integral in (2.1.50) extends also over the center interval and therefore, of necessity, is very large. For example,

$$\left\{\int_0^1 g_n(t;\mathrm{d}\lambda)\,\mathrm{d}\ell(t)\right\}^{1/2} \doteq 2.0\times 10^9 \quad \text{if } n=40,$$

and hence the same large magnitude for the condition number $(\operatorname{cond}\widetilde{\boldsymbol{G}}_n)(\widetilde{\boldsymbol{m}})$. Clearly, the "hole" $[\frac{1}{3},\frac{2}{3}]$ must be avoided at all cost. A possibility in this regard, suggested by Wheeler (1984), is

$$\mathrm{d}\ell(t)=\begin{cases} 18\pi^{-1}|t-\frac{1}{2}|^{-1}\{t(1-t)(t-\frac{1}{3})(t-\frac{2}{3})\}^{1/2}\,\mathrm{d}t, & t\in[0,\frac{1}{3}]\cup[\frac{2}{3},1],\\ 0 & \text{otherwise,}\end{cases} \tag{2.1.133}$$

for which the corresponding modified moments as well as the polynomials $p_k = p_k(\,\cdot\,;\mathrm{d}\ell)$ are explicitly computable (Wheeler, 1984). The polynomial g_n being, of course, the same as before, one now has

$$(\operatorname{cond}\widetilde{\boldsymbol{G}}_n)(\widetilde{\boldsymbol{m}})=\left\{\int_{[0,\frac{1}{3}]\cup[\frac{2}{3},1]} g_n(t;\mathrm{d}\lambda)\,\mathrm{d}\ell(t)\right\}^{1/2} < 1 \tag{2.1.134}$$

for all n, in striking contrast with the previous choice of $\mathrm{d}\ell$.

The last example is one in which the modified Chebyshev algorithm fails.

Example 2.31 The *half-range Hermite* measure $\mathrm{d}\lambda(t)=\mathrm{e}^{-t^2}\,\mathrm{d}t$ on $[0,\infty]$.

We apply the modified Chebyshev algorithm with two choices of modified moments, the first relative to monic Hermite polynomials, $p_k^H = 2^{-k}H_k$, the second relative to monic Laguerre polynomials, $p_k^L=(-1)^k k!L_k$ (cf. Commentary to Table 1.1). The respective recursion coefficients are

$$a_k=0\ (k\ge 0);\quad b_0=\sqrt{\pi},\ b_k=\tfrac{1}{2}k\ (k\ge 1)\quad \text{(Hermite)} \tag{2.1.135}$$

and

$$a_k=2k+1\ (k\ge 0);\quad b_0=1,\ b_k=k^2\ (k\ge 1)\quad \text{(Laguerre)}. \tag{2.1.136}$$

For the Hermite moments $m_k^H=\int_0^\infty p_k^H(t)\mathrm{e}^{-t^2}\,\mathrm{d}t$, one finds from the recurrence relation for the Hermite polynomials, integration by parts, and from the identity $H_k'=2kH_{k-1}$, that

$$\begin{aligned} m_k^H &= \tfrac{1}{2}\,p_{k-1}^H(0),\quad k=1,2,\ldots,\\ m_0^H &= \tfrac{1}{2}\sqrt{\pi}. \end{aligned} \tag{2.1.137}$$

Here, $p_{k-1}^H(0)=0$ if k is even, and $p_{k-1}^H(0)=(-1)^{(k-1)/2}(k-1)!/2^{k-1}((k-1)/2)!$ if k is odd. The latter can be computed recursively. The modified Chebyshev

algorithm furnished with the data in (2.1.135) and (2.1.137) performs as shown in Table 2.7 in a format similar to the one in Table 2.6. (High-accuracy values of the $\alpha_k(\mathrm{d}\lambda)$ and $\beta_k(\mathrm{d}\lambda)$ were obtained in quadruple precision by methods discussed in §2.2. The first 100 of them are available to 25 decimal places in the `OPQ` file `abhrhermite`.) It seems natural, here, to show the relative condition numbers of (2.1.64), although the absolute condition numbers of (2.1.50) are almost the same, but consistently a bit larger.

It is seen that the modified Chebyshev algorithm becomes quickly unstable,

Table 2.7 *Condition number and error magnification for the half-range Hermite measure using Hermite moments.*

n	(2.1.64)	$\operatorname{mag}\alpha$	$\operatorname{mag}\beta$
2	1.94(1)	1.50(0)	5.00(–1)
4	4.60(3)	1.21(2)	3.75(1)
6	1.67(6)	3.15(3)	3.65(3)
8	6.79(8)	4.81(6)	1.69(6)
10	2.91(11)	2.62(9)	1.10(9)

though not quite as fast as predicted by the condition numbers.

For the Laguerre moments $m_k^L = \int_0^\infty p_k^L(t)\mathrm{e}^{-t^2}\,\mathrm{d}t$, one finds from the explicit power representation of the Laguerre polynomials that[1]

$$m_k^L = \frac{(-1)^k k!}{2} \sum_{\rho=0}^{k} (-1)^\rho \frac{k!\Gamma((\rho+1)/2)}{(k-\rho)!\rho!^2}, \quad k = 0, 1, 2, \ldots . \tag{2.1.138}$$

The terms in the sum for ρ even and for ρ odd can be generated recursively from initial values $\sqrt{\pi}$ resp. $-k$.

With these Laguerre moments, and the data in (2.1.136), the modified Chebyshev algorithm, surprisingly, is found to perform worse than with Hermite moments, in spite of the fact that the Laguerre measure has support identical to the one of $\mathrm{d}\lambda$, unlike the Hermite measure. The latter, however, has a stronger damping power as $|x| \to \infty$, which probably accounts for its better performance in the modified Chebyshev algorithm. The results are shown in Table 2.8.

Tables 2.7 and 2.8 are computed with the `OPQ` routines `Table2_7.m` and `Table2_8.m`.

As Example 2.31 demonstrates, there are limitations in the potential usefulness of moment-related methods, particularly for measures $\mathrm{d}\lambda$ having unbounded support. Fortunately, there are other methods available that work also in these

[1]Equation (5.29) in Gautschi (1984c) contains a misprint: the factor $k!$ in the summation on the far right should be $k!^2$.

Table 2.8 *Condition number and error magnification for the half-range Hermite measure using Laguerre moments.*

n	(2.1.64)	mag α	mag β
2	9.54(1)	2.70(1)	3.75(–1)
4	2.41(6)	2.56(6)	5.63(4)
6	2.99(11)	2.15(11)	7.20(9)
8	8.73(16)	1.40(17)	6.28(15)
10	5.45(22)	1.40(17)	6.10(18)

difficult circumstances, although they may be more labor-intensive and also require a certain amount of creativity on the part of the user. These will be discussed in the next section.

2.2 Discretization methods

The basic idea behind discretization methods is very simple. One approximates the given measure $\mathrm{d}\lambda$ by a discrete N-point measure $\mathrm{d}\lambda_N$, computes the recursion coefficients $\alpha_{k,N} = \alpha_k(\mathrm{d}\lambda_N)$, $\beta_{k,N} = \beta_k(\mathrm{d}\lambda_N)$ of the discrete measure $\mathrm{d}\lambda_N$, and then lets N go to infinity. If the discretizations are done in a meaningful manner, the process will converge in the sense that, for fixed k, $\lim_{N\to\infty} \alpha_{k,N} = \alpha_k$ and $\lim_{N\to\infty} \beta_{k,N} = \beta_k$, where $\alpha_k = \alpha_k(\mathrm{d}\lambda)$ and $\beta_k = \beta_k(\mathrm{d}\lambda)$ are the desired recursion coefficients of the given measure. There are, however, a number of issues—some theoretical and some practical—that need to be considered. The first concerns the question of convergence, the second the problem of computing recursion coefficients of discrete measures, and the third and most important one, appropriate choices of discretizations. These issues will be discussed in turn in §2.2.1–2.2.4. Nontrivial examples illustrating the power of these methods will be given in §2.2.5. The same apparatus of discretization, created to approximate inner products, can be applied to approximate modified moments instead, which, in combination with the modified Chebyshev algorithm, then provides another approach toward computing recursion coefficients. This will be briefly discussed in §2.2.6.

2.2.1 *Convergence of discrete orthogonal polynomials to continuous ones*

We first assume that the measure $\mathrm{d}\lambda$ is supported on a finite interval, say $[-1, 1]$, and that the support points of $\mathrm{d}\lambda_N$ are also contained in $[-1, 1]$.

It is reasonable to expect that the discrete orthogonal polynomials $\pi_{n,N}(\,\cdot\,) = \pi_n(\,\cdot\,; \mathrm{d}\lambda_N)$ converge to the continuous orthogonal polynomials $\pi_n(\,\cdot\,) = \pi_n(\,\cdot\,; \mathrm{d}\lambda)$ as $N \to \infty$ if the inner product

$$(p, q)_{\mathrm{d}\lambda_N} := \int_{\mathbb{R}} p(t)q(t)\,\mathrm{d}\lambda_N(t) = \sum_{\nu=1}^{N} w_\nu p(t_\nu)q(t_\nu) \tag{2.2.1}$$

(where t_ν and w_ν depend on N) converges to $(p,q)_{\mathrm{d}\lambda}$ as $N \to \infty$ whenever p and q are polynomials. This is borne out by the following theorem.

Theorem 2.32 *Let* $\mathrm{d}\lambda$ *be a positive measure on* $[-1,1]$ *having finite moments of all orders* (cf. §1.1.1) *and* $\mathrm{d}\lambda_N$ *the discrete measure (2.2.1) with* $t_\nu = t_{\nu,N}$ *distinct numbers in* $[-1,1]$ *and* $w_\nu = w_{\nu,N} > 0$ *for each* N. *Assume that*

$$\lim_{N\to\infty} (p,q)_{\mathrm{d}\lambda_N} = (p,q)_{\mathrm{d}\lambda} \quad \text{if } p \in \mathbb{P},\ q \in \mathbb{P}, \tag{2.2.2}$$

where $\mathbb{P}$ *is the class of real polynomials. Then, for any fixed* k, *the recursion coefficients* $\alpha_{k,N}$ *and* $\beta_{k,N}$ *for the discrete orthogonal polynomials relative to the measure* $\mathrm{d}\lambda_N$ *converge to those of the continuous orthogonal polynomials,*

$$\lim_{N\to\infty} \alpha_{k,N} = \alpha_k, \quad \lim_{N\to\infty} \beta_{k,N} = \beta_k, \tag{2.2.3}$$

where $\alpha_k = \alpha_k(\mathrm{d}\lambda)$, $\beta_k = \beta_k(\mathrm{d}\lambda)$. *Furthermore,*

$$\lim_{N\to\infty} \pi_n(t;\mathrm{d}\lambda_N) = \pi_n(t;\mathrm{d}\lambda) \tag{2.2.4}$$

uniformly for t *in* $[-1,1]$.

Proof The proof is based on the formulae (cf. Theorem 1.27)

$$\alpha_k = \frac{(t\pi_k,\pi_k)_{\mathrm{d}\lambda}}{(\pi_k,\pi_k)_{\mathrm{d}\lambda}}, \quad k = 0,1,2,\ldots, \tag{2.2.5}$$

$$\beta_k = \frac{(\pi_k,\pi_k)_{\mathrm{d}\lambda}}{(\pi_{k-1},\pi_{k-1})_{\mathrm{d}\lambda}}, \quad k = 1,2,\ldots, \tag{2.2.6}$$

where $\pi_k(\,\cdot\,) = \pi_k(\,\cdot\,;\mathrm{d}\lambda)$ are the (monic) orthogonal polynomials relative to $\mathrm{d}\lambda$, and the corresponding formulae

$$\alpha_{k,N} = \frac{(t\pi_{k,N},\pi_{k,N})_{\mathrm{d}\lambda_N}}{(\pi_{k,N},\pi_{k,N})_{\mathrm{d}\lambda_N}}, \quad k = 0,1,2,\ldots, \tag{2.2.7}$$

$$\beta_{k,N} = \frac{(\pi_{k,N},\pi_{k,N})_{\mathrm{d}\lambda_N}}{(\pi_{k-1,N},\pi_{k-1,N})_{\mathrm{d}\lambda_N}}, \quad k = 1,2,\ldots, \tag{2.2.8}$$

for the discrete polynomials. By definition,

$$\beta_0 = (1,1)_{\mathrm{d}\lambda}, \quad \beta_{0,N} = (1,1)_{\mathrm{d}\lambda_N}. \tag{2.2.9}$$

We begin with the observation that for any $f, g \in C[-1,1]$ there holds

$$|(f,g)_{\mathrm{d}\lambda_N}| \le \|f\|_\infty \|g\|_\infty (1,1)_{\mathrm{d}\lambda_N}, \tag{2.2.10}$$

where the infinity norm is the one with respect to the interval $[-1,1]$.

Proceeding by induction on n, assume that (2.2.4) is true for some $n = s$ and $n = s-1$. (This is trivial when $s = 0$.) In order to prove (2.2.4) for $n = s+1$, it

suffices to prove (2.2.3) for $k = s$ since this, by the three-term recurrence relation $\pi_{s+1,N}(t) = (t-\alpha_{s,N})\pi_{s,N}(t) - \beta_{s,N}\pi_{s-1,N}(t)$ and the induction hypothesis, will imply $\pi_{s+1,N}(t) \to (t-\alpha_s)\pi_s(t) - \beta_s\pi_{s-1}(t) = \pi_{s+1}(t)$. In order to prove (2.2.3), on the other hand, it suffices to show that all the inner products appearing in (2.2.7) and (2.2.8), when $k = s$, converge to the corresponding ones in (2.2.5) and (2.2.6) as $N \to \infty$. We show this for the inner product $(\pi_{s,N}, \pi_{s,N})_{\mathrm{d}\lambda_N}$; for the others, the proof is analogous.

We have

$$\begin{aligned}(\pi_{s,N}, \pi_{s,N})_{\mathrm{d}\lambda_N} &= (\pi_s + (\pi_{s,N} - \pi_s), \pi_s + (\pi_{s,N} - \pi_s))_{\mathrm{d}\lambda_N} \\ &= (\pi_s, \pi_s)_{\mathrm{d}\lambda_N} + 2(\pi_s, \pi_{s,N} - \pi_s)_{\mathrm{d}\lambda_N} + (\pi_{s,N} - \pi_s, \pi_{s,N} - \pi_s)_{\mathrm{d}\lambda_N}.\end{aligned} \tag{2.2.11}$$

The first term on the far right, by (2.2.2), converges to $(\pi_s, \pi_s)_{\mathrm{d}\lambda}$. To the second term we apply (2.2.10) with the result that

$$|(\pi_s, \pi_{s,N} - \pi_s)_{\mathrm{d}\lambda_N}| \le \|\pi_s\|_\infty \|\pi_{s,N} - \pi_s\|_\infty (1,1)_{\mathrm{d}\lambda_N}.$$

Since by assumption $(1,1)_{\mathrm{d}\lambda_N} \to (1,1)_{\mathrm{d}\lambda}$ and by the induction hypothesis, $\pi_{s,N} \to \pi_s$, the bound on the right tends to zero. By the same reasoning, the last term in (2.2.11) also tends to zero. Consequently,

$$\lim_{N\to\infty} (\pi_{s,N}, \pi_{s,N})_{\mathrm{d}\lambda_N} = (\pi_s, \pi_s)_{\mathrm{d}\lambda}.$$

□

Note that according to the last relation in the proof of Theorem 2.32, one has $\|\pi_{n,N}\|_{\mathrm{d}\lambda_N} \to \|\pi_n\|_{\mathrm{d}\lambda}$, which, combined with (2.2.4), shows that Theorem 2.32 also holds for ortho*normal* polynomials (cf. §1.3.2), that is,

$$\lim_{N\to\infty} \tilde{\pi}_n(t; \mathrm{d}\lambda_N) = \tilde{\pi}_n(t; \mathrm{d}\lambda). \tag{2.2.12}$$

Theorem 2.32 has the following simple corollary.

Corollary to Theorem 2.32 Let n be fixed and the zeros of π_n, in decreasing order, be denoted by $\tau_1, \tau_2, \ldots, \tau_n$ and those of $\pi_{n,N}$, in the same order, by $\tau_{1,N}, \tau_{2,N}, \ldots, \tau_{n,N}$. Then, under the assumptions of Theorem 2.32, there holds

$$\lim_{N\to\infty} \tau_{\nu,N} = \tau_\nu, \quad \lim_{N\to\infty} \pi_{m,N}(\tau_{\nu,N}) = \pi_m(\tau_\nu), \quad \nu = 1, 2, \ldots, n;\ m \ne n. \tag{2.2.13}$$

Proof The first relation in (2.2.13) is a consequence of the continuity of polynomial zeros. The second relation follows from

$$\pi_{m,N}(\tau_{\nu,N}) - \pi_m(\tau_\nu) = (\pi_{m,N}(\tau_{\nu,N}) - \pi_m(\tau_{\nu,N})) + (\pi_m(\tau_{\nu,N}) - \pi_m(\tau_\nu))$$

by observing that $|\pi_{m,N}(\tau_{\nu,N}) - \pi_m(\tau_{\nu,N})| \le \|\pi_{m,N} - \pi_m\|_\infty \to 0$ and $\pi_m(\tau_{\nu,N}) \to \pi_m(\tau_\nu)$ as $N \to \infty$. □

Remark The first relation in (2.2.13) can be interpreted by saying that the nodes of the n-point Gauss quadrature rule for $\mathrm{d}\lambda_N$ (cf. §1.4.2) tend to the nodes of the n-point Gauss quadrature rule for $\mathrm{d}\lambda$. The same holds also for the respective weights $\lambda^G_{\nu,N}$ and λ^G_ν. This follows by applying the second relation in (2.2.13) (for orthonormal polynomials) to the formula (cf. eqn (3.1.7))

$$\lambda^G_{\nu,N} = \frac{1}{\sum_{m=0}^{n-1} \tilde{\pi}^2_{m,N}(\tau_{\nu,N})}, \quad \nu = 1, 2, \ldots, n. \tag{2.2.14}$$

2.2.2 *A general-purpose discretization procedure*

Discretizations $(p,q)_{\mathrm{d}\lambda_N}$ of $(p,q)_{\mathrm{d}\lambda}$ as in (2.2.1) can be obtained by applying suitable quadrature formulae. We illustrate this in the case $\mathrm{d}\lambda(t) = w(t)\,\mathrm{d}t$, where w is continuous on $(-1,1)$ but may have integrable singularities at ± 1. We seek an approximation of the form

$$\int_{-1}^{1} f(t)w(t)\,\mathrm{d}t \cong \sum_{\nu=1}^{N} w_\nu f(t_\nu)w(t_\nu), \tag{2.2.15}$$

which can then be used, with $f(t) = p(t)q(t)$, to obtain the discrete inner product (2.2.1). There are of course other possibilities, for example, *weighted* quadrature rules $\int_{-1}^{1} f(t)w(t)\,\mathrm{d}t \cong \sum_{\nu=1}^{N} w_\nu f(t_\nu)$, the construction of which, however, will depend on the particular nature of the weight function w. The choice (2.2.15) is made with the intention in mind of providing a general-purpose discretization. Since w may be singular at the end points ± 1, the nodes t_ν are preferably chosen away from these points unless one wants to play the risky game of "ignoring" the singularity (cf. Davis and Rabinowitz (1984, §2.12.7)). Moreover, a high degree of exactness is desirable whenever w happens to be smooth on $[-1,1]$. This suggests to use an interpolatory quadrature rule (cf. §1.4.1) and nodes t_ν that are denser near the end points ± 1; for example, exhibiting an arccos-distribution. A quadrature rule that fits this bill is the interpolatory quadrature rule based on the Chebyshev points, also called the *Fejér quadrature rule*. Thus, its nodes are

$$t^F_\nu = \cos\theta^F_\nu, \quad \theta^F_\nu = \frac{2\nu - 1}{2N}\,\pi, \quad \nu = 1, 2, \ldots, N, \tag{2.2.16}$$

and its weights are explicitly known,

$$w^F_\nu = \frac{2}{N}\left(1 - 2\sum_{n=1}^{\lfloor N/2 \rfloor} \frac{\cos 2n\theta^F_\nu}{4n^2 - 1}\right), \quad \nu = 1, 2, \ldots, N. \tag{2.2.17}$$

Fejér (1933) indeed has shown that $w^F_\nu > 0$ for all ν, and, therefore, by a well-known theorem of Pólya (cf. Davis and Rabinowitz (1984, p. 130)), the Fejér quadrature rule converges for continuous functions. In particular, (2.2.15) with $t_\nu = t^F_\nu$, $w_\nu = w^F_\nu$, converges as $N \to \infty$ whenever f is a polynomial and w

continuous on $[-1,1]$. Interestingly, convergence persists even if w has integrable singularities at ± 1 provided w is monotonic nearby (Gautschi, 1967b). Little is known, however, about the rate of convergence in such cases, and it may well be that convergence is quite slow (cf. Example 2.33). Fejér quadrature rules are generated in the `OPQ` routine `fejer.m`.

If $\mathrm{d}\lambda$ contains also a discrete component, it suffices to add this component to the discrete approximation of the absolutely continuous part of $\mathrm{d}\lambda$. This does not affect in any way the convergence properties of the discretization.

An arbitrary support interval $[a,b]$, $-\infty \le a < b \le \infty$, can be reduced to the canonical interval $[-1,1]$ by a suitable transformation of variables,

$$\int_a^b f(t)w(t)\,\mathrm{d}t = \int_{-1}^1 f(\phi(\tau))w(\phi(\tau))\phi'(\tau)\,\mathrm{d}\tau. \tag{2.2.18}$$

If $[a,b]$ is finite, a linear transformation will do, otherwise a simple fractional transformation. In our work, we have used

$$\phi(\tau) = \begin{cases} \frac{1}{2}(b-a)\tau + \frac{1}{2}(b+a) & \text{if } -\infty < a < b < \infty, \\ b - \dfrac{1-\tau}{1+\tau} & \text{if } -\infty = a < b < \infty, \\ a + \dfrac{1+\tau}{1-\tau} & \text{if } -\infty < a < b = \infty, \\ \dfrac{\tau}{1-\tau^2} & \text{if } -\infty = a < b = \infty. \end{cases} \tag{2.2.19}$$

The `OPQ` routine `quadgp.m` in combination with the routine `fejer.m` provides the quadrature nodes and weights for use in (2.2.18) if one applies the Fejér rule to the integral on the right.

Such transformations, in fact, can be useful also if, in an attempt to speed up convergence, one decides to partition the interval $[a,b]$ into a number of subintervals and to apply Fejér quadrature to each one of them. But how should such a partition be produced? Here is a systematic way of going about it. Assume, for the sake of argument, that the singularity lies at the left end point a and that b is a regular point. Suppose also that we are trying to achieve a result with error $\le \varepsilon$ and are willing to use Fejér rules with as many as $N_{\max}$ points, but not more, on each subinterval. Pick a t_1^0 with $a < t_1^0 < b$ (and fairly close to a). Apply the n-point Fejér rule to the interval $[a,t_1^0]$ with $n = 2,3,\ldots$ and monitor the absolute value of the difference bewtween two successive approximations to the integral. If this difference becomes $\le \varepsilon$ for some $n < N_{\max}$, increase t_1^0 to t_1^1 and try again on the interval $[a,t_1^1]$. Otherwise, decrease t_1^0 and repeat until the error condition can be satisfied with $n < N_{\max}$. Eventually, a t_1 will be found for which the Fejér rule with about $N_{\max}$ points applied to $[a,t_1]$ yields the desired accuracy. We accept t_1 as the first point of the partition. The same process is then repeated on some interval $[t_1,t_2^0]$, $t_1 < t_2^0 \le b$, to produce the second point

t_2 of the partition, and so on. The process terminates once the right end point of a subinterval reaches the end point b.

Example 2.33 $f(t) = 1$ and $w(t) = t^t(1-t)^{1-t}$ on $[0,1]$.

By the symmetry $w(1-t) = w(t)$, it suffices to compute

$$\int_0^1 w(t)\,\mathrm{d}t = 2\int_0^{1/2} w(t)\,\mathrm{d}t. \tag{2.2.20}$$

With the choice $\varepsilon = \frac{1}{2}10^{-14}$ and $N_{\max} = 50$, the partition procedure described above, when applied to $[0,1/2]$, produces the partition $[0,0.5] = [0,0.00115] \cup [0.00115,0.0844] \cup [0.0844,0.5]$. Applying the composite Fejér rule on this partition, using n quadrature points on each subinterval until an $n = N$ is reached for which the total error is $\leq \varepsilon$ yields $N = 108$ (in Matlab) with the result having an error of 0.4996×10^{-14}. (Quadruple-precision computation of the integral yields the value $0.617826964729011473\ldots$, which was used as a reference value for computing errors.) The fact that N is rather larger than $N_{\max}$ may at first surprise, but on reflection (and testing) can be ascribed to the more rigorous testing against the exact result as opposed to comparing two consecutive approximations, as was done in the generation of the partition. In contrast, applying the Fejér rule with $N = 108$ and $N = 3 \times 108 = 324$ over the whole interval $[0,1/2]$ yields 0.6178269656443711 resp. 0.6178269647402954 with errors 0.9154×10^{-9} and 0.1128×10^{-10}. The partition of the interval thus proves to be beneficial in this example. See the `OPQ` routine `Example2_33.m` for details.

Example 2.34 The integral $\int_0^\infty \mathrm{e}^{-t^2}\,\mathrm{d}t = \frac{1}{2}\sqrt{\pi}$.

Here, $f(t) = 1$ and w is the half-range Hermite weight function. With the same choice of ε as in Example 2.33, but $N_{\max} = 20$, the partition becomes $[0,\infty] = [0,1.013] \cup [1.013,3.639] \cup [3.639,\infty]$, on which the Fejér composite rule with $N = 22$ points on each subinterval yields the desired accuracy ε. See the `OPQ` routine `Example2_34.m`

2.2.3 *Computing the recursion coefficients of a discrete measure*

We discuss two procedures, one already briefly alluded to by Stieltjes (1884, p. 415 or p. 383 of Œuvres, Vol. I) in 1884, and another implementing ideas of Lanczos and Rutishauser.

2.2.3.1 *Stieltjes procedure* The formulae (2.2.7) and (2.2.8) for the recursion coefficients provide a natural framework for computing them. All inner products

$$(p,q)_{\mathrm{d}\lambda_N} = \sum_{\nu=1}^{N} w_\nu p(t_\nu) q(t_\nu) \tag{2.2.21}$$

appearing in these formulae indeed are finite sums and therefore trivial to compute. The only problem is the appearance of the polynomials $\pi_{k,N}$ and $\pi_{k-1,N}$ themselves, which are not known. However, they can be built up successively, and

in tandem with the recursion coefficients, by the three-term recurrence relation (cf. §1.3.1).

$$\pi_{k+1,N}(t) = (t - \alpha_{k,N})\pi_{k,N}(t) - \beta_{k,N}\pi_{k-1,N}(t), \quad k = 0, 1, \ldots, N-1. \tag{2.2.22}$$

Since $\pi_{0,N} = 1$, the coefficient $\alpha_{0,N}$ indeed can be computed from (2.2.7) with $k = 0$, and so can $\beta_{0,N} = (1,1)_{\mathrm{d}\lambda_N}$. This allows us to compute $\pi_{1,N}(t)$, for all values $t = t_\nu$ needed, by means of (2.2.22) with $k = 0$. In possession of the values $\pi_{1,N}(t_\nu)$ and $\pi_{0,N}(t_\nu)$, the formulae (2.2.7) and (2.2.8) now become applicable and yield $\alpha_{1,N}$ and $\beta_{1,N}$. This, in turn, can be used in (2.2.22) to generate $\pi_{2,N}$. In this manner, alternating between (2.2.22) and (2.2.7), (2.2.8), we can proceed until all recursion coefficients, or as many as are needed, have been computed. The procedure is implemented in the `OPQ` routine `stieltjes.m`.

The procedure is not entirely foolproof, numerically. For one, there is some danger of overflow or underflow occurring during the course of the procedure. This may happen for one of two reasons: over- resp. underflow of the weights w_ν, or over- resp. underflow of the orthogonal polynomials $\pi_{k,N}$ or, more precisely, of their squared norms. A remedy in the former case is to multiply all weights by a sufficiently large resp. small number c prior to running the procedure. In the latter case, a scaling of the polynomials is required, which is most easily accomplished by multiplying $\pi_{0,N}$ by c (assuming $\pi_{-1,N} = 0$). In either case, the recursion coefficients remain the same except for $\beta_{0,N}$, which, at the end, must be divided by c.

A potentially more serious problem is the tendency of the recurrence relation (2.2.22) to develop instabilities as k approaches N. The phenomenon—a type of *pseudostability*—has been pointed out and analyzed in Gautschi (1993b), (1997a, §3.4.2). If it occurs, and it is likely to do so if the support points $t_{\nu,N}$ are equally, or nearly equally, spaced, then the numerical performance of the Stieltjes procedure is seriously impaired in its advanced stages. Nevertheless, in applications such as discretization methods it is usually the case that N is much larger than the number of recursion coefficients to be computed. The problem of pseudostability then need not be of any concern.

Example 2.35 The *discrete Chebyshev polynomials*, revisited.

The Stieltjes procedure is applied to generate the (known) recursion coefficients $\alpha_{n,N}$ and $\beta_{n,N}$ of the equally spaced and equally weighted discrete measure of Example 2.26. The results, produced by the `OPQ` routine `Table2_9.m`, are shown in Table 2.9. The columns headed $\mathrm{err}\,\alpha$ and $\mathrm{err}\,\beta$ display the absolute errors in the α- and β-coefficients for selected values of n and, at the bottom of each record, the largest errors taken over all n, $0 \le n \le N-1$.

As is evident from these results, when N is large, a good portion of the higher-order coefficients $\alpha_{n,N}$ and $\beta_{n,N}$ has extremely poor accuracy, the relative size of this portion growing with N.

The example also provides an illustration of the underflow problem mentioned above: when $N = 320$, the squared norms of the polynomials $\pi_{k,N}$ were found

Table 2.9 *Errors in the recursion coefficients of discrete Chebyshev polynomials computed by the Stieltjes procedure.*

N	n	err α	err β	N	n	err α	err β
40	≤ 37	$\leq 1.0(-14)$	$\leq 1.0(-14)$	160	82	2.143(–15)	3.490(–15)
	38	2.577(–13)	3.370(–15)		89	8.978(–11)	1.208(–11)
	39	1.932(–11)	1.257(–13)		96	8.466(–07)	1.026(–07)
		1.932(–11)	1.257(–13)		103	1.874(–02)	2.195(–03)
80	≤ 55	$\leq 1.0(-14)$	$\leq 1.0(-14)$			1.952(–01)	7.075(–02)
	56	1.266(–14)	1.422(–15)	320	≤ 115	$\leq 1.0(-14)$	$\leq 1.0(-14)$
	60	2.478(–11)	1.769(–12)		116	2.287(–14)	3.990(–15)
	64	9.651(–08)	5.504(–09)		127	1.238(–10)	2.204(–11)
	68	1.197(–03)	5.132(–05)		138	1.768(–06)	2.967(–07)
		2.756(–01)	5.650(–02)		149	3.483(–02)	7.498(–03)
160	≤ 81	$\leq 1.0(-14)$	$\leq 1.0(-14)$			1.416(–01)	6.224(–02)

to underflow beginning around $k = 245$. The results of Table 2.9, in this case, were obtained by scaling the polynomials by the factor $c = 10^{50}$.

We add another, more favorable, example lest the reader dismisses Stieltjes's procedure as untrustworthy.

Example 2.36 The *discrete Fejér measure* on $[-1, 1]$, that is, the inner product (2.2.21) in which $t_\nu = t_\nu^F$, $w_\nu = w_\nu^F$ are the Fejér nodes and weights (2.2.16), (2.2.17).

As demonstrated by the `OPQ` routine `Table2_10.m`, using the same values of N as in Table 2.9, the results of Stieltjes's procedure are now perfect in all respects. The maximum errors for each N are shown in Table 2.10. (Reference values to 18 decimal places for the β-coefficients are available in the `OPQ` files `befej40`–`befej320`.)

Table 2.10 *Maximum errors in the recursion coefficients of discrete Fejér polynomials computed by the Stieltjes procedure.*

N	err α	err β
40	2.585(–15)	1.055(–15)
80	3.088(–15)	1.388(–15)
160	6.594(–15)	2.442(–15)
320	1.254(–14)	4.829(–15)

Example 2.36 provides additional support for the use of Fejér quadrature in discretization processes when no better and more natural alternatives are available.

2.2.3.2 *A Lanczos-type algorithm* Given a real symmetric matrix $\boldsymbol{A}$, there exists an orthogonal similarity transformation $\boldsymbol{Q}^{\mathrm{T}}\boldsymbol{A}\boldsymbol{Q} = \boldsymbol{T}$ to a tridiagonal sym-

metric matrix $\boldsymbol{T}$ having nonnegative elements on the two side diagonals. In general, the orthogonal matrix $\boldsymbol{Q}$ and the matrix $\boldsymbol{T}$ are uniquely determined by $\boldsymbol{A}$ and the first column of $\boldsymbol{Q}$ (cf. Parlett (1998, §7-2)). *Lanczos's algorithm* (see also §3.1.7.1) is a method that produces $\boldsymbol{Q}$ and $\boldsymbol{T}$, given $\boldsymbol{A}$.

With the nodes t_ν and positive weights w_ν of the discrete inner product (2.2.1), we form the vector $\sqrt{\boldsymbol{w}}$ and diagonal matrix $\boldsymbol{D}_t$ defined by

$$\sqrt{\boldsymbol{w}} = \begin{bmatrix} \sqrt{w_1} \\ \sqrt{w_2} \\ \vdots \\ \sqrt{w_N} \end{bmatrix}, \quad \boldsymbol{D}_t = \begin{bmatrix} t_1 & 0 & \cdots & 0 \\ 0 & t_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & t_N \end{bmatrix}. \tag{2.2.23}$$

Then, it is true (cf. §3.1.1.1) that there exists an orthogonal matrix $\boldsymbol{Q}_1$ of order N such that

$$\begin{bmatrix} 1 & \boldsymbol{0}^{\mathrm{T}} \\ \boldsymbol{0} & \boldsymbol{Q}_1^{\mathrm{T}} \end{bmatrix} \begin{bmatrix} 1 & \sqrt{\boldsymbol{w}}^{\mathrm{T}} \\ \sqrt{\boldsymbol{w}} & \boldsymbol{D}_t \end{bmatrix} \begin{bmatrix} 1 & \boldsymbol{0}^{\mathrm{T}} \\ \boldsymbol{0} & \boldsymbol{Q}_1 \end{bmatrix} = \begin{bmatrix} 1 & \sqrt{\beta_{0,N}}\boldsymbol{e}_1^{\mathrm{T}} \\ \sqrt{\beta_{0,N}}\boldsymbol{e}_1 & \boldsymbol{J}_N(\mathrm{d}\lambda_N) \end{bmatrix}, \tag{2.2.24}$$

where $\boldsymbol{e}_1^{\mathrm{T}} = [1, 0, \ldots, 0] \in \mathbb{R}^N$ and $\boldsymbol{J}_N(\mathrm{d}\lambda_N)$ is the Nth-order Jacobi matrix (cf. Definition 1.30) of the discrete measure $\mathrm{d}\lambda_N$ in (2.2.1). Thus, we are in the situation described in the opening paragraph of this subsection, where

$$\boldsymbol{A} = \begin{bmatrix} 1 & \sqrt{\boldsymbol{w}}^{\mathrm{T}} \\ \sqrt{\boldsymbol{w}} & \boldsymbol{D}_t \end{bmatrix}, \quad \boldsymbol{Q} = \begin{bmatrix} 1 & \boldsymbol{0}^{\mathrm{T}} \\ \boldsymbol{0} & \boldsymbol{Q}_1 \end{bmatrix}, \tag{2.2.25}$$

and $\boldsymbol{T}$ is the "extended" Jacobi matrix on the right of (2.2.24). The nonzero elements of the latter are precisely the recursion coefficients $\alpha_{k,N}$ and $\beta_{k,N}$ that we wish to determine. Since $\boldsymbol{A}$ is given, and so is the first column $\boldsymbol{e}_1 \in \mathbb{R}^{N+1}$ of $\boldsymbol{Q}$, the Lanczos algorithm can, in principle, be applied to compute the desired recursion coefficients. We say "in principle" since, unfortunately, the process is numerically unstable. A stable variant, however, following ideas of Rutishauser (1963), has been developed by Gragg and Harrod (1984), who use a sequence of Givens rotations to construct the orthogonal similarity transformation in (2.2.24). The construction is summarized in their pseudocode RKWW, which we transcribed into Matlab to produce the `OPQ` routine `lanczos.m`.

Example 2.37 This repeats Example 2.35 with the routine `lanczos.m` used in place of `stieltjes.m`.

It is found that all errors, when $N = 40, 80, 160, 320$, are now bounded, respectively, by 4.996×10^{-16}, 1.554×10^{-15}, 2.554×10^{-15}, and 5.773×10^{-15}. Thus, in this example, `lanczos.m` is vastly superior to `stieltjes.m` in terms of accuracy. Timings, however, reveal that `lanczos.m` is about eight times slower than `stieltjes.m`. For details, see the `OPQ` routine `Example2_37.m`.

There are instances in which Stieltjes's procedure outperforms the Lanczos algorithm outright; some are described in Examples 2.40 and 2.44 of §2.2.5.

2.2.4 *A multiple-component discretization method*

We begin with an example intended to motivate the seemingly complicated procedure to be described later in this section.

Example 2.38 Chebyshev weight function plus a constant, $w(t;c) = (1-t^2)^{-1/2} + c$ on $[-1,1]$, $c > 0$; see also Example 3.45.

What quadrature rule should be used to discretize $w(t;c)$? It would be difficult to come up with one that can be applied over the whole interval $[-1,1]$ and would converge reasonably fast. The Fejér rule, for example, when $c = 1$, requires 690 points to integrate $w(\,\cdot\,;1)$ just to get three correct decimal places, and the Gauss–Legendre rule even more. Factoring out $(1-t^2)^{-1/2}$ and applying Gauss–Chebyshev quadrature to the rest, $1 + c(1-t^2)^{1/2}$, works better, yielding three decimal places with 29 points, but still requires 287 points to get five decimal places. (See the `OPQ` routine `Example2_38.m`.) Clearly, it is more expedient to discretize the two parts of the weight function separately and combine the results. Thus, one treats the first term, $(1-t^2)^{-1/2}$, as a weight function and applies Gauss–Chebyshev quadrature to the function 1, and then applies Gauss–Legendre quadrature to the constant c to deal with the second term. Taking M points in each quadrature and adding the results yields an N-point discretization with $N = 2M$ which is exact for all M, even for $M = 1$.

In the context of generating the recursion coefficients $\beta_k(w)$ of $w(\,\cdot\,;c)$ (all $\alpha_k(w) = 0$) by the Stieltjes procedure, one needs to integrate not only w but also polynomials against the weight function w. The degree of these polynomials is at most $2n-1$ if we are interested in the first n coefficients $\beta_0, \beta_1, \ldots, \beta_{n-1}$. The choice $M = n$ in the proposed procedure then performs all integrations exactly by virtue of the two quadrature rules being Gauss rules. This means that the $2n$-point discrete inner product generated by the procedure has recursion coefficients $\beta_{k,2n}(w)$, $k = 0, 1, \ldots, n-1$, which are identical with the corresponding coefficients β_k of w that we set out to determine. We can compute them by either the Stieltjes procedure or the Lanczos algorithm as described in §2.2.3.

As an aside, note that the orthogonal polynomials relative to the weight function $w(\,\cdot\,;c)$ (which, to the best of our knowledge, are not explicitly known) may be thought of as "interpolating" between the Chebyshev polynomials ($c = 0$) and the Legendre polynomials ($c = \infty$). It is interesting, therefore, to observe the behavior of the coefficients $\beta_k(w(\,\cdot\,;c))$, $k \geq 1$, as a function of c. (The first coefficient is $\beta_0 = \pi + 2c$ and has no resemblance with the corresponding coefficient $\beta_0 = 2$ for Legendre polynomials.) Graphs of the first four coefficients are shown in Fig. 2.2; they are produced by the `OPQ` routine `Figure2_2.m`.

Example 2.38 suggests the idea of decomposing the given measure $\mathrm{d}\lambda$ into one with *multiple components*. Thus, if $\mathrm{d}\lambda(t) = w(t)\,\mathrm{d}t$ is absolutely continuous, for example, and has support $[a,b]$, $-\infty \leq a < b \leq \infty$, then the interval $[a,b]$ is decomposed into a union of m subintervals,

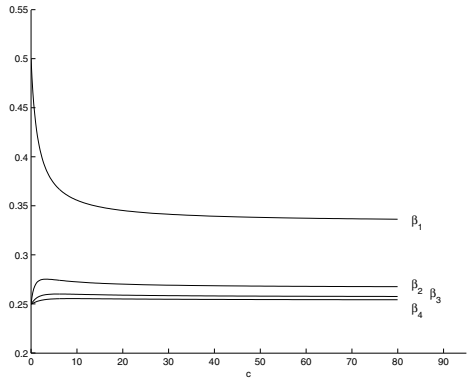

FIG. 2.2. Recursion coefficients for the weight function $w(\,\cdot\,;c)$ of Example 2.38, $0 \le c \le 80$.

$$[a,b] = \bigcup_{\mu=1}^{m} [a_\mu, b_\mu], \quad m \ge 1, \tag{2.2.26}$$

which may or may not be disjoint, and each subinterval is endowed with its own weight function w_μ, which may or may not be identical with w. More precisely, the integral of a polyomial f against the measure $\mathrm{d}\lambda$ is represented in the form

$$\int_a^b f(t)w(t)\,\mathrm{d}t = \sum_{\mu=1}^{m} \int_{a_\mu}^{b_\mu} f_\mu(t)w_\mu(t)\,\mathrm{d}t, \tag{2.2.27}$$

where we allowed for the possibility that f_μ differs from f and may depend on μ; in fact, f_μ may no longer be a polynomial but is assumed to be a smooth function. It may also be the case that the union of intervals in (2.2.26) differs from $[a,b]$ (see, e.g. Example 2.44).

A simple illustration of (2.2.27) is provided by Example 2.38, where the weight function w on $[a,b]$ is a sum of two weight functions, $w = w_1 + w_2$. In this case, $m = 2$, and the two intervals $[a_\mu, b_\mu]$ are both equal to $[a,b]$, but the first carries the weight function w_1 and the second w_2. Alternatively, one may simply want to partition the interval $[a,b]$ into smaller subintervals as in Examples 2.33 and 2.34, and keep the original weight function w the same in all subintervals. Yet another scenario is the situation in which the original weight function has multiple support intervals to begin with; these can then be taken as the intervals $[a_\mu, b_\mu]$ in (2.2.26) or can be decomposed still further. In all these cases, f_μ is the same as f. There are examples, however, where this is no longer true (see Examples 2.40, 2.44, and 2.45).

Now in order to discretize (2.2.27), one applies a quadrature rule to each constituent integral on the right. Depending on the nature of the weight function w_μ, the rule could be a weighted quadrature, such as a Gauss rule relative to the weight function w_μ, or the general-purpose Fejér rule as in §2.2.2. If one takes the

same number M of nodes in each quadrature rule, one ends up with an N-point discretization of (2.2.27) with $N = mM$. If the original measure $\mathrm{d}\lambda$, in addition to the absolutely continuous component has also a discrete p-point component, one simply adds on this component and extends the (mM)-point discretization to an $(mM + p)$-point discretization.

The multiple-component discretization procedure now consists in the following. Apply discretizations of the type described with a monotone increasing sequence $M_0, M_1, M_2, \ldots$ of M-values to obtain discrete measures $\mathrm{d}\lambda_{mM_i+p}$, $i = 0, 1, 2, \ldots$. For each i, compute by one of the methods of §2.2.3 the discrete recursion coefficients $\alpha_k^{[i]} = \alpha_{k,mM_i+p}$, $\beta_k^{[i]} = \beta_{k,mM_i+p}$ for $k = 0, 1, \ldots, n-1$, where n is the number of recursion coefficients desired. Continue until the process converges. A convenient measure for convergence is the relative error in the β-coefficients, since they are all positive. Thus, the iteration is stopped at the first value of $i \geq 1$ for which

$$|\beta_k^{[i]} - \beta_k^{[i-1]}| \leq \varepsilon \beta_k^{[i]}, \quad k = 0, 1, 2, \ldots, n-1, \tag{2.2.28}$$

where ε is a given error tolerance. In view of (2.2.7) and (2.2.8), it is reasonable to expect, and in fact is borne out by experience, that satisfaction of (2.2.28) entails sufficient accuracy also for the α-coefficients $\alpha_k^{[i]}$—absolute accuracy if they are zero or small, and relative accuracy otherwise.

It remains to elaborate on the choice of the sequence $\{M_i\}$. Through a bit of experimentation, we have settled on the following sequence:

$$\begin{aligned} &M_i = M_0 + \Delta_i, \quad i = 1, 2, 3, \ldots, \\ &\Delta_1 = 1, \quad \Delta_i = 2^{\lfloor i/5 \rfloor} \cdot n, \quad i = 2, 3, \ldots . \end{aligned} \tag{2.2.29}$$

The default value of M_0 is $M_0 = 2n$. However, one can do better. If the quadrature rules used in the discretization process all have algebraic degree of exactness $\geq d(M)$ with $d(M)/M = \delta + O(M^{-1})$ as $M \to \infty$, then taking $M_0 = 1 + \lfloor (2n-1)/\delta \rfloor$ may well give exact answers after one iteration. This is the case, for example, when all quadrature rules are Gauss rules, hence $\delta = 2$, in which case $M_0 = n$ and the process terminates after one iteration. An instance of this has been noted in Example 2.38. For interpolatory quadratures, one has $\delta = 1$, giving $M_0 = 2n$, the default value of M_0.

The procedure described is implemented in the `OPQ` routine `mcdis.m`. It outputs not only the desired recursion coefficients, but also `Mcap`, the value of M_i that achieves convergence, and `kount`, the corresponding number of iterations.

2.2.5 *Examples*

In this section, we demonstrate the considerable power inherent in the multiple-component discretization method as a means for generating orthogonal polynomials even relative to measures that are unconventional and highly nontrivial. In a number of examples it will be shown how to take advantage of the flexibility

built into the method in order to achieve efficiency and accuracy. At the same time, comparisons will be made between the multiple-component discretization method used with the Stieltjes procedure and used with Lanczos's algorithm.

Example 2.39 *Jacobi weight function plus a discrete measure.*

The measure to be considered is the normalized Jacobi weight function on $[-1, 1]$ with a discrete p-point measure added to it,

$$\mathrm{d}\lambda(t) = [\beta_0^J]^{-1}(1-t)^\alpha(1+t)^\beta\,\mathrm{d}t + \sum_{j=1}^{p} y_j\delta(t-t_j)\,\mathrm{d}t, \quad \alpha > -1,\ \beta > -1,\ y_j > 0. \tag{2.2.30}$$

Here, $\beta_0^J = \int_{-1}^{1}(1-t)^\alpha(1+t)^\beta\,\mathrm{d}t$ and $\delta(\,\cdot\,)$ is the Dirac delta function. The orthogonal polynomials belonging to the measure (2.2.30) are explicitly known only in very special cases. The case of one mass point at one end point, that is, $p = 1$ and $t_1 = -1$, has been studied by Chihara (1985, §6(E)), who managed to express the recursion coefficients in terms of the classical ones for the Jacobi weight function.[2] The formulae are rather complicated; see, for example, Gautschi (1994, eqns (4.19)–(4.21)). Adding a second mass at the other end point makes the analytical determination of the recursion coefficients virtually intractable, although analytic expressions of the orthogonal polynomials themselves in terms of hypergeometric functions are still known (Koornwinder, 1984). Any kind of analytic treatment, however, will become quite unfeasible if further masses are added, inside and/or outside the interval $[-1, 1]$. It is, therefore, all the more remarkable that, numerically, it makes no difference how many mass points there are and where they are located. The procedure is always the same: discretize the continuous part of the measure by the appropriate Gauss–Jacobi quadrature, add on the discrete part, and then use either the Stieltjes or Lanczos algorithm, as described in §2.2.3, to generate the recursion coefficients of the discretized measure. If we need n of each and use n-point Gauss–Jacobi quadrature, then, as noted at the end of §2.2.4, the answers turn out to be the exact recursion coefficients of (2.2.30) and no iteration is required. We found, however, that Stieltjes's procedure becomes extremely unstable if one or more mass points are located outside the interval $[-1, 1]$. In this case, the use of Lanczos's algorithm is imperative.

The `OPQ` routine `r_jacplusdis.m` generates the recursion coefficients of (2.2.30) for arbitrary values of the parameters subject to the conditions stated.

Table 2.11, computed by the `OPQ` routine `Table2_11.m`, illustrates the performance of the procedure in the case of one mass point of various strengths located at the left end point -1. We generate 40 recursion coefficients for 100 values $\alpha = -0.8(0.2)1.0$, $\beta = -0.8(0.2)1.0$ of the Jacobi parameters, and with masses $y_1 = 0.5, 2, 10$. In each run, we produce two results, one using Stieltjes's

[2]Chihara takes the interval $[0, 2]$ rather than $[-1, 1]$. There appears to be a typo in the first formula of his eqn (6.23), which should have the numerator $2\beta + 2$ instad of $2\beta + 1$.

Table 2.11 *Stieltjes procedure vs Lanczos algorithm in the multiple-component method for Example 2.39 with one mass point at $t = -1$.*

y	n	α_n	β_n	discr α	discr β
0.5	0	3.7037037037(–2)	1.5000000000(+0)	1.18(–16)	0.00(+00)
	6	3.2391629514(–2)	2.3060042904(–1)	1.39(–17)	1.11(–16)
	17	4.4564744879(–3)	2.4754733005(–1)	2.13(–16)	3.89(–16)
	39	8.6966173737(–4)	2.4953594220(–1)	7.05(–16)	3.61(–16)
				5.24(–15)	1.55(–15)
2	0	–4.8148148148(–1)	3.0000000000(+0)	1.67(–16)	1.48(–16)
	6	3.2967435170(–2)	2.3019023360(–1)	1.21(–15)	8.33(–17)
	17	4.4611147047(–3)	2.4754467376(–1)	1.76(–15)	3.89(–16)
	39	8.6975321827(–4)	2.4953589362(–1)	1.85(–15)	2.78(–16)
				4.78(–15)	1.47(–15)
10	0	–8.5858585859(–1)	1.1000000000(+1)	3.33(–16)	1.61(–16)
	6	3.3122514092(–2)	2.3007952696(–1)	5.41(–16)	0.00(+00)
	17	4.4623528161(–3)	2.4754396497(–1)	3.80(–16)	4.16(–16)
	39	8.6977761461(–4)	2.4953588066(–1)	5.57(–17)	3.33(–16)
				4.37(–15)	1.42(–15)

procedure and the other using the Lanczos algorithm, and determine their discrepancy. (By discrepancy between two answers we mean their absolute or relative difference, as the answer is ≤ 1 resp. >1 in modulus.) The table shows the recursion coefficients $\alpha_n(\mathrm{d}\lambda)$ and $\beta_n(\mathrm{d}\lambda)$ for $\alpha = -0.6$, $\beta = 0.4$ to 10 decimal places for selected values of n, followed by their discrepancies. At the bottom of each record, the maximum discrepancy is shown, where the maximum is taken over all $n = 0, 1, 2, \ldots, 39$ and all 100 Jacobi parameters. It can be seen that the Stieltjes and Lanczos algorithms produce essentially identical results within machine precision, although Lanczos is about eight times slower.

The results are very much alike if a second mass point is added at the end point $+1$, or yet a third one at the origin (see the routine `Table2_11.m`). Matters change significantly (see the `OPQ` routine `Table2_12.m`) when a mass point is placed outside $[-1, 1]$, regardless of whether or not the other mass points on $[-1, 1]$ are retained. This is illustrated in Table 2.12 for a single mass point of strength $y_1 = 1$ at $t = 2$. Since we allowed only one iteration in the multiple-component discretization method (in theory, this yields exact answers), the routine `mcdis.m`, when using Stieltjes's procedure (`irout`=1), returns with the message that the error criterion could not be achieved. No such message is issued when the Lanczos algorithm is used. The reason for this must be attributed to the instability phenomenon, already mentioned in §2.2.3.1, inherent in Stieltjes's procedure, and this also explains the large values of the discrepancies seen in Table 2.12.

Example 2.40 The *generalized Jacobi measure*.

This is the measure

Table 2.12 *Stieltjes procedure vs Lanczos algorithm in the multiple-component method for Example 2.39 with one mass point at $t = 2$.*

y	n	α_n	β_n	discr α	discr β
1	0	1.2777777778(+0)	2.0000000000(+0)	0.00(+00)	0.00(+00)
	6	–1.9575723334(–3)	2.4959807576(–1)	3.07(–16)	2.78(–16)
	17	–1.9175655273(–4)	2.4998241443(–1)	2.48(–15)	4.72(–16)
	39	–3.4316341540(–5)	2.4999770643(–1)	2.37(–06)	7.60(–07)
				1.00(+00)	7.50(–01)

$$\mathrm{d}\lambda(t) = (1-t)^{\alpha}(1+t)^{\beta}\prod_{\mu=2}^{m}|t-t_\mu|^{\gamma_\mu}\,\mathrm{d}t, \quad \alpha > -1,\ \beta > -1, \tag{2.2.31}$$

on $[-1,1]$, where $m \geq 2$, $-1 < t_2 < \cdots < t_m < 1$, and γ_μ are nonzero parameters with $\gamma_\mu > -1$. Some authors include a smooth factor $\varphi(t)$ in the definition of the generalized Jacobi measure, but in the context of numerical quadrature φ can be absorbed by the integrand function f. If one defines $t_1 = -1$, $t_{m+1} = 1$ and correspondingly $\gamma_1 = \beta$, $\gamma_{m+1} = \alpha$, one can write

$$\mathrm{d}\lambda(t) = \prod_{\nu=1}^{m+1}|t-t_\nu|^{\gamma_\nu}\,\mathrm{d}t.$$

This suggests the decomposition

$$[-1,1] = \bigcup_{\mu=1}^{m}[t_\mu, t_{\mu+1}],$$

and integration of a polynomial f against the measure $\mathrm{d}\lambda$ takes the form

$$\int_{-1}^{1} f(t)\,\mathrm{d}\lambda(t) = \sum_{\mu=1}^{m}\int_{t_\mu}^{t_{\mu+1}} f(t)\prod_{\substack{\nu=1\\ \nu\neq\mu;\nu\neq\mu+1}}^{m+1}|t-t_\nu|^{\gamma_\nu}\,w_\mu(t)\,\mathrm{d}t, \tag{2.2.32}$$

where

$$w_\mu(t) = (t_{\mu+1}-t)^{\gamma_{\mu+1}}(t-t_\mu)^{\gamma_\mu}, \quad t_\mu < t < t_{\mu+1}, \tag{2.2.33}$$

is a Jacobi weight function on the interval $[t_\mu, t_{\mu+1}]$ with parameters $\gamma_{\mu+1}$, γ_μ. The representation (2.2.32) is precisely of the form (2.2.27): on each interval $[t_\mu, t_{\mu+1}]$, instead of the polynomial f one must integrate the function f_μ obtained from f by multiplication with the product appearing on the right of (2.2.32). It is clear, then, how the inner product $(p,q)_{\mathrm{d}\lambda}$ must be discretized: apply a Gauss–Jacobi quadrature relative to the interval $[t_\mu, t_{\mu+1}]$, with Jacobi parameters $\gamma_{\mu+1}$ and γ_μ, to each integral on the right of (2.2.32), where $f = pq$. This, in general, will no longer produce exact answers as in the previous example since the product in (2.2.32) is not a polynomial. However, convergence can be expected to be quite fast; see Tables 2.13–2.14.

The OPQ routine `r_gjacobi.m` implements this procedure and generates the recursion coefficients of the measure (2.2.31) for any parameters satisfying the conditions stated.

As a test example for `r_gjacobi.m`, we took the simple case $m = 2$, $\alpha = \beta = -1/2$, $t_2 = 0$, $\gamma_2 = 1$. By symmetry, all $\alpha_k(\mathrm{d}\lambda)$ vanish, and $\beta_k(\mathrm{d}\lambda)$ can be determined explicitly. Indeed, consider the polynomials p_k^+ and p_k^- defined by $\pi_{2k}(t) = p_k^+(t^2)$, $\pi_{2k+1}(t) = tp_k^-(t^2)$ (cf. Theorem 1.18). One easily checks that these are (ordinary) Jacobi polynomials relative to the interval $[0, 1]$, in fact $p_k^+(x) = G_k(\frac{1}{2}, 1, x)$, $p_k^-(x) = G_k(\frac{3}{2}, 2, x)$ in the notation of Abramowitz and Stegun (1992, 22.2.2). Writing the recurrence relation $\pi_{2k+1}(t) = t\pi_{2k}(t) - \beta_{2k}\pi_{2k-1}(t)$ in terms of p_k^+ and p_k^-, one finds $tp_k^-(t^2) = tp_k^+(t^2) - \beta_{2k}tp_{k-1}^-(t^2)$; hence,

$$\beta_{2k} = \frac{p_k^+(t^2) - p_k^-(t^2)}{p_{k-1}^-(t^2)} \to c_k^+ - c_k^- \quad \text{as } t \to \infty, \quad k \geq 1,$$

where c_k^+ and c_k^- are the coefficients of x^{k-1} in $p_k^+(x)$ and $p_k^-(x)$, respectively. From 22.3.3 of Abramowitz and Stegun (1992), these are $c_k^+ = k^2/(2k - 1/2)$ resp. $c_k^- = k(k + 1)/(2k + 1/2)$. There follows

$$\beta_{2k}(\mathrm{d}\lambda) = k\,\frac{k - 1/2}{4k^2 - 1/4}\,, \quad k \geq 1. \tag{2.2.34}$$

Similarly, one finds

$$\beta_{2k+1}(\mathrm{d}\lambda) = (k + 1)\frac{k + 1/2}{(2k + 1)^2 - 1/4}\,, \quad k \geq 0. \tag{2.2.35}$$

The OPQ routine `gjactest.m` calls on `r_gjacobi.m` to compute the first N recursion coefficients, $N = 10, 40, 80, 160$, for the test example. It determines the maximum absolute error in the α-coefficients and the maximum relative error of the β-coefficients, and also prints the integers `Mcap`, `kount` from the routine `mcdis.m`, which give an indication of the convergence behavior of the multiple-component discretization method (for the error tolerance `eps0`=1000×`eps`). The results are shown in Table 2.13. Convergence is seen to be very fast, and in fact

Table 2.13 *Results for the test example.*

N	Mcap	kount	err α	err β
10	31	3	1.494(–15)	2.911(–15)
40	41	1	5.938(–16)	4.323(–15)
80	81	1	1.229(–15)	9.150(–15)
160	161	1	4.881(–15)	1.915(–14)

is achieved after one iteration when $N \geq 40$. The accuracy is as good as can be hoped for. The results shown are those obtained using Stieltjes's procedure; Lanczos yields essentially the same answers but is about eight times slower.

To illustrate our procedure on a more elaborate example, we consider the (t, γ)-configuration

t	–1	–1/2	0	1/2	1
γ	–1/2	1/3	1	–1/3	1/2

and use `r_gjacobi.m` to generate the first 160 recursion coefficients. Selected values of these coefficients are shown in Table 2.14 together with the corresponding discrepancies (between the Stieltjes and Lanczos results). Shown at the bottom of the table are the maximum discrepancies taken over all values $n = 0, 1, 2, \ldots, 159$. (For details, see the `OPQ` routine `Table2_14.m`.) The multiple-component discretization method, run with an error tolerance `eps0`=1000×`eps`, converged in one iteration exiting with an M-value (cf. (2.2.29)) of $M = 161$. Difficulties must be expected if some of the t_μ are bunched together very closely, as, for example, in the "crowding" phenomenon in Schwarz–Christoffel mappings (Driscoll and Trefethen, 2002, §2.6).

Table 2.14 *Stieltjes procedure vs Lanczos algorithm in the multiple-component method for Example 2.40.*

n	α_n	β_n	discr α	discr β
0	7.2811345991(–1)	3.2069708827(+0)	1.11(–16)	0.00(+00)
39	–4.4829921025(–3)	2.4184615756(–1)	9.01(–15)	1.67(–16)
79	–2.2131034661(–3)	2.4727751247(–1)	4.73(–15)	2.78(–17)
119	–3.2863129782(–3)	2.4909284690(–1)	5.33(–15)	3.89(–16)
159	–1.1138360928(–3)	2.4796821583(–1)	5.67(–15)	2.78(–17)
			1.06(–14)	1.61(–15)

Example 2.41 The *half-range Hermite* measure $\mathrm{d}\lambda(t) = \mathrm{e}^{-t^2}\,\mathrm{d}t$ on $[0, \infty]$, revisited.

We have seen in Example 2.31 that for this measure moment-related methods are ineffective. Discretization is here a more viable alternative, even though there are no special features of the measure that would suggest particularly natural discretizations. We therefore use the general-purpose discretization based on Fejér quadrature, but decompose the inverval into four subintervals, $[0, \infty] = [0, 3] \cup [3, 6] \cup [6, 9] \cup [9, \infty]$ (obtained by trial and error). This is implemented in the `OPQ` routine `r_hrhermite.m` and run by the routine `Table2_15.m` with `N`=40, `Mmax`=100, and `eps0`=1000×`eps`. The multiple-component discretization routine `mcdis.m` returns with output parameters `Mcap`=81, `kount`=1, indicating convergence after one iteration. The results are displayed in Table 2.15, where the errors err α and err β are obtained by comparison with quadruple-precision results available to 25 decimal places in the `OPQ` file `abhrhermite`.

Table 2.15 *The multiple-component method (with Stieltjes's procedure) applied to Example 2.41.*

n	α_n	β_n	err α	err β
0	5.6418958355(–1)	8.8622692545(–1)	5.55(–16)	2.22(–16)
1	9.8842539285(–1)	1.8169011382(–1)	1.78(–15)	1.67(–16)
6	2.0806203364(+0)	1.0023478510(+0)	6.40(–16)	0.00(+00)
15	3.2142706361(+0)	2.5009279171(+0)	4.14(–16)	1.78(–16)
26	4.2030485789(+0)	4.3338679012(+0)	2.32(–15)	2.05(–16)
39	5.1315328869(+0)	6.5003562377(+0)	2.42(–15)	5.47(–16)
			3.02(–15)	1.33(–15)

Example 2.42 *Einstein and Fermi distributions.*

Distributions frequently encountered in solid state physics are the Einstein distribution

$$\mathrm{d}\lambda(t) = \varepsilon(t)\,\mathrm{d}t, \quad \varepsilon(t) = \frac{t}{\mathrm{e}^t - 1} \quad \text{on } [0,\infty],$$

and the Fermi distribution

$$\mathrm{d}\mu(t) = \varphi(t)\,\mathrm{d}t, \quad \varphi(t) = \frac{1}{\mathrm{e}^t + 1} \quad \text{on } [0,\infty],$$

as well as distributions involving powers of ε and φ,

$$\mathrm{d}\lambda^{[r]}(t) = [\varepsilon(t)]^r\,\mathrm{d}t, \quad \mathrm{d}\mu^{[r]}(t) = [\varphi(t)]^r\,\mathrm{d}t, \quad r \geq 1.$$

Table 2.16 *Recurrence coefficients for Einstein measures computed by the discretization method.*

r	n	$\alpha_n(\mathrm{d}\lambda^{[r]})$	$\beta_n(\mathrm{d}\lambda^{[r]})$	err α	err β
1	4	9.8286605540(0)	1.9473894450(1)	1.81(–16)	7.30(–16)
	9	1.9881441597(1)	8.9117330865(1)	2.50(–15)	2.07(–15)
	19	3.9916946226(1)	3.7862460617(2)	5.34(–16)	4.65(–15)
				2.50(–15)	4.65(–15)
2	4	5.2618141802(0)	5.6467693899(0)	2.19(–15)	1.26(–15)
	9	1.0334264562(1)	2.4163978775(1)	1.89(–15)	2.79(–15)
	19	2.0383323902(1)	9.8826669339(1)	0.00(+00)	1.44(–15)
				3.02(–15)	5.85(–15)

With regard to the Einstein distribution, a natural discretization of the inner product $(u,v)_{\mathrm{d}\lambda^{[r]}}$ can be obtained by writing the respective integrals in the form

$$\int_0^\infty p(t)\,\mathrm{d}\lambda^{[r]}(t) = \int_0^\infty p(t)\left(\frac{t}{\mathrm{e}^t-1}\right)^r \mathrm{d}t = \frac{1}{r}\int_0^\infty p(t/r)\left(\frac{t/r}{1-\mathrm{e}^{-t/r}}\right)^r \mathrm{e}^{-t}\,\mathrm{d}t$$

(where $p = uv$) and applying M-point Gauss–Laguerre quadrature to the integral on the right. To obtain the first $n = 20$ recursion coefficients $\alpha_k(\mathrm{d}\lambda^{[r]})$,

$\beta_k(\mathrm{d}\lambda^{[r]})$, $k = 0, 1, \ldots, n-1$, to an accuracy of about 14 decimal digits (`eps0`= $100\times$`eps`$\approx 2.22 \times 10^{-14}$) requires $M = 121$ for $r = 1$ and $M = 81$ for $r = 2$; see the `OPQ` routine `Example2_42.m`. Selected results, with respective errors and maximum errors, are shown in Table 2.16. The (mollified) errors (cf. the paragraph preceding Example 2.14) are computed by comparison with quadruple-precision results available to 25 decimal places in the `OPQ` files `abeinstein1` and `abeinstein2`.

The results for the two Fermi distributions $\mathrm{d}\mu^{[r]}$, $r = 1, 2$, are quite similar except that it takes larger values of M to achieve the same accuracy—M=161 and M=121, respectively. The reason for this is the location of the poles of φ, which are twice as close to the real axis compared to the poles of ε. See `Example2_42.m` for numerical results and `abfermi1`, `abfermi2` for quadruple-precision values of $\alpha_k(\mathrm{d}\mu^{[r]})$, $\beta_k(\mathrm{d}\mu^{[r]})$, $r = 1, 2$.

Example 2.43 *Modified Einstein and Fermi distributions.*

In applications to slowly convergent series (cf. §3.4, Examples 3.63 and 3.68–3.69), it is required to deal with Einstein and Fermi distributions modified by square-root factors,

$$\mathrm{d}\tilde{\lambda}_{\pm}^{[r]}(t) = t^{\pm 1/2}\,\mathrm{d}\lambda^{[r]}(t), \quad \mathrm{d}\tilde{\mu}_{\pm}^{[r]}(t) = t^{\pm 1/2}\,\mathrm{d}\mu^{[r]}(t) \quad \text{on } [0,\infty]. \tag{2.2.36}$$

In this case, the discretization used in Example 2.42 has to be modified to take account of the square-root singularity at $t = 0$. It was found convenient to split the interval $[0,\infty)$ into two parts, $[0, 10]$ and $[10,\infty)$, and apply Gauss–Jacobi quadrature with parameters $\alpha = 0$, $\beta = \pm\frac{1}{2}$ on the first, and Gauss–Laguerre quadrature on the second interval. This works rather well, the values of M required being $M = 61$ in all cases. Results for the modified Einstein distributions $\mathrm{d}\tilde{\lambda}_{+}^{[r]}$, analogous to those in Table 2.16, are shown in Table 2.17. For modified Fermi distributions, the results are very similar; see the `OPQ` routine `Example2_43.m`. Quadruple-precision values of the first 80 recursion coeffi-

Table 2.17 *Recurrence coefficients for modified Einstein measures computed by a two-component discretization method.*

r	n	$\alpha_n(\mathrm{d}\tilde{\lambda}_{+}^{[r]})$	$\beta_n(\mathrm{d}\tilde{\lambda}_{+}^{[r]})$	err α	err β
1	4	1.0334741121(1)	2.1678201766(1)	5.16(–16)	0.00(+00)
	9	2.0383465049(1)	9.3837339797(1)	1.22(–15)	1.06(–15)
	19	4.0417639589(1)	3.8835425850(2)	2.99(–15)	5.85(–16)
				2.99(–15)	5.26(–15)
2	4	5.5191016116(0)	6.2493698392(0)	2.57(–15)	1.42(–15)
	9	1.0586711541(1)	2.5398321854(1)	0.00(+00)	1.12(–15)
	19	2.0634174813(1)	1.0131580628(2)	5.17(–16)	1.54(–15)
				3.44(–15)	2.94(–15)

cients, stored in the files `absqp1einstein1`, `absqp1einstein2`, `absqp1fermi1`, and `absqp1fermi2`, were used to compute the errors.

Example 2.44 *Logistic density function*

$$w(t) = \frac{\mathrm{e}^{-t}}{(1+\mathrm{e}^{-t})^2}\,, \quad -\infty < t < \infty. \tag{2.2.37}$$

Logistic density and distribution functions are widely used in applied statistics; see, for example, Johnson et al. (1995, Chapter 23). Integrals involving the weight function w are required in order to compute expected values of functions relative to the logistic distribution. A representation of the type (2.2.27) for such integrals is obtained in a natural way by splitting the integral into two parts, one from $-\infty$ to 0 and the other from 0 to ∞, and changing variables in the first part. The result is

$$\int_{-\infty}^{\infty} f(t)w(t)\,\mathrm{d}t = \int_0^{\infty} \frac{f(-t)}{(1+\mathrm{e}^{-t})^2}\,w_1(t)\,\mathrm{d}t + \int_0^{\infty} \frac{f(t)}{(1+\mathrm{e}^{-t})^2}\,w_1(t)\,\mathrm{d}t, \tag{2.2.38}$$

where $w_1(t) = \mathrm{e}^{-t}$ is the Laguerre weight function. Since $(1+\mathrm{e}^{-t})^2$ tends rapidly to 1 as $t \to \infty$, the two integrals on the right are best discretized by applying Gauss–Laguerre quadrature to the functions $f(\mp t)(1+\mathrm{e}^{-t})^{-2}$. The performance of the multiple-component discretization method can be easily tested since the recursion coefficients are explicitly known: all $\alpha_k(\mathrm{d}\lambda) = 0$ by symmetry, and $\beta_0 = 1$, $\beta_k(\mathrm{d}\lambda) = k^4\pi^2/(4k^2-1)$, $k \geq 1$; see Chihara (1978, eqn (8.7)) where $\lambda = 0$, $x = t/\pi$. Table 2.18 (computed by the `OPQ` routine `Table2_18.m`) shows selected results when the routine `mcdis.m` is run with `N`=40 and `eps0`=1000×`eps`, and with Stieltjes's procedure used to compute the recursion coefficients. (Lanczos's algorithm gives essentially the same results but takes about 10 times as long.) Again, the maximum errors are shown at the bottom of the table.

Table 2.18 *The multiple-component discretization method applied to Example 2.44.*

n	β_n	err α	err β
0	1.0000000000(0)	7.18(–17)	3.33(–16)
1	3.2898681337(0)	1.29(–16)	2.70(–16)
6	8.9447603523(1)	4.52(–16)	1.43(–15)
15	5.5578278399(2)	2.14(–14)	0.00(+00)
26	1.6685802223(3)	1.23(–14)	6.81(–16)
39	3.7535340252(3)	6.24(–14)	4.48(–15)
		6.24(–14)	8.75(–15)

Example 2.45 A *weight function involving a modified Bessel function*,

$$w(t) = t^{\alpha}K_0(t) \;\text{ on } [0,\infty], \quad \alpha > -1. \tag{2.2.39}$$

The recursion coefficients for this weight function can be used to generate associated Gauss quadrature rules (cf. §3.1.1), which in turn are useful to obtain

asymptotic approximations to oscillatory integral transforms (Wong, 1982). The choice of decomposition and discretization appropriate here should reflect, and make optimal use of, the special properties of the weight function $w(t)$, especially its behavior for small and large t. This can be done by observing that

$$K_0(t) = \begin{cases} R(t) + I_0(t)\ln(1/t) & \text{if } 0 < t \le 1, \\ t^{-1/2}\mathrm{e}^{-t}S(t) & \text{if } 1 \le t < \infty, \end{cases} \tag{2.2.40}$$

where I_0 is the "regular" modified Bessel function and R, S are well-behaved smooth functions for which good rational approximations are available (Russon and Blair, 1969). This leads naturally to a decomposition $[0,\infty] = [0,1] \cup [0,1] \cup [0,\infty]$ and

$$\begin{aligned} \int_0^\infty f(t)w(t)\,\mathrm{d}t = &\int_0^1 [R(t)f(t)]t^\alpha\,\mathrm{d}t + \int_0^1 [I_0(t)f(t)]t^\alpha \ln(1/t)\,\mathrm{d}t \\ &+ \mathrm{e}^{-1}\int_0^\infty [(1+t)^{\alpha-1/2}S(1+t)f(1+t)]\mathrm{e}^{-t}\,\mathrm{d}t. \end{aligned} \tag{2.2.41}$$

Thus, in the notation of (2.2.27),

$$f_1(t) = R(t)f(t), \quad w_1(t) = t^\alpha \text{ on } [0,1],$$

$$f_2(t) = I_0(t)f(t), \quad w_2(t) = t^\alpha \ln(1/t) \text{ on } [0,1],$$

$$f_3(t) = \mathrm{e}^{-1}(1+t)^{\alpha-1/2}S(1+t)f(1+t), \quad w_3(t) = \mathrm{e}^{-t} \text{ on } [0,\infty].$$

The appropriate discretization, therefore, is Gauss–Jacobi quadrature (with parameters 0 and α) of f_1 on $[0,1]$, Gauss quadrature of f_2 relative to the weight function w_2 on $[0,1]$, and Gauss–Laguerre quadrature of f_3 on $[0,\infty]$. While the first and last quadratures are classical, the middle one is not, but can be accurately generated by methods discussed in §3.1.1 once the recursion coefficients for w_2 are known. These, in turn, can be computed by means of the modified Chebyshev algorithm as described in Example 2.27.

The `OPQ` routine `r_modbess.m` implements this procedure for arbitrary parameter α.

As an illustration, we consider the integral (cf. Gradshteyn and Ryzhik (2000, 6.621.3))

$$\int_0^\infty \mathrm{e}^{-t}t^\alpha K_0(t)\,\mathrm{d}t = \frac{\sqrt{\pi}}{2^{\alpha+1}}\,\frac{\Gamma^2(\alpha+1)}{\Gamma(\alpha+3/2)}\,.$$

The routine `Table2_19.m` uses `r_modbess.m` to obtain Gauss quadrature approximations to this integral for selected values of α, requesting an accuracy of $10^5\texttt{eps} = 2.22 \times 10^{-11}$. The number n of Gauss points required is shown in Table 2.19. The maximum relative error observed is 3.21×10^{-12}.

Table 2.19 *Gauss quadrature of a Bessel function integral.*

α	–0.9	–0.5	0	0.8	2.3	5.8
n	10	12	13	14	15	18

2.2.6 *Discretized modified Chebyshev algorithm*

We note that the idea of multiple-component discretization, embodied in eqn (2.2.27), and subsequent discretizations of the subintegrals on the right of (2.2.27) can be used to approximate any integral $\int_{\mathbb{R}} f(t)\,\mathrm{d}\lambda(t)$. In the discretization method of §2.2.4, the integral in question is an inner product, $f(t) = p(t)q(t)$, and the discretization procedure is used to approximate the inner product $(p,q)_{\mathrm{d}\lambda}$ by a multiple-component discrete inner product $(p,q)_{\mathrm{d}\lambda_{mM}}$ (or more generally $(p,q)_{\mathrm{d}\lambda_{mM+p}}$ if $\mathrm{d}\lambda$ contains a p-point discrete measure); cf. the second paragraph following eqn (2.2.27). The same procedure, however, could also be applied to approximate modified moments, $m_r = \int_{\mathbb{R}} p_r(t)\,\mathrm{d}\lambda(t)$, in the modified Chebyshev algorithm. Here, $f(t) = p_r(t)$ (cf. (2.1.23)). Thus, one constructs a sequence of discretizations, as in §2.2.4, with M-values $M_0, M_1, M_2, \ldots$, and for each i applies the modified Chebyshev algorithm using discretized modified moments $m_r^{[i]} = \int_{\mathbb{R}} p_r(t)\,\mathrm{d}\lambda_{mM_i+p}$ to generate approximate recursion coefficients $\alpha_k^{[i]}$, $\beta_k^{[i]}$. The same stopping criterion (2.2.28) as before can be used to terminate the iteration. In fact, it is essential that convergence be tested on the βs and not, for example, on the modified moments, since the latter may vanish and, besides, need not be required to have full relative precision (see Gautschi (1982b, p. 311)). The procedure is implemented in the `OPQ` routine `mcchebyshev.m`.

It is important to realize, however, that any ill-conditioning present in the modified Chebyshev algorithm must be expected to manifest itself also in its discretized version. There are fewer such problems with discretization procedures based on inner products.

Example 2.46 Example 2.29, revisited.

We have seen in Example 2.29 that computing exact values of modified moments (relative to Chebyshev polynomials) for the "elliptic" weight function $w(t) = [(1-k^2t^2)(1-t^2)]^{-1/2}$ can be highly nontrivial. Approximate values, on the other hand, can easily be obtained via the Gauss–Chebyshev quadrature rule

$$\int_{-1}^{1} f(t)(1-k^2t^2)^{-1/2}(1-t^2)^{-1/2}\,\mathrm{d}t \approx \frac{\pi}{M}\sum_{m=1}^{M} f(t_m)(1-k^2t_m^2)^{-1/2},$$

where $t_m = \cos((2m-1)\pi/2M)$, by applying it with $f(t) = 2^{1-r}T_r(t)$ resp. $f(t) = 1$ to compute the modified moment m_r, $r \geq 1$, resp. m_0. The discretized modified Chebyshev algorithm, run with $k^2 = 0.1, 0.5, 0.9$, and 0.999, and with $N = 40$, using the error tolerance `eps0`$= 1000\times$`eps`, produces results essentially identical with those of Example 2.29; see the `OPQ` routine `Example2_46.m`.

2.3 Computing Cauchy integrals of orthogonal polynomials

Cauchy's theorem in the theory of complex variables expresses the value of an analytic function at some point z by means of a contour integral extended over a simple closed curve in the complex plane encircling the point z. The type of integral involved is referred to as a *Cauchy integral*. The same integral is also of interest if the function on the contour is not analytic and/or the contour is not a closed curve but an open arc. One continues to call such integrals Cauchy integrals. There is a vast literature on them and their applications; see, for example, Henrici (1986, Chapter 14). Here we are interested in Cauchy integrals over an interval on the real line involving a positive measure of integration $\mathrm{d}\lambda$ and the orthogonal polynomial $\pi_n(\,\cdot\,;\mathrm{d}\lambda)$ associated with this measure. Thus,

$$(\mathcal{C}\pi_n)(z;\mathrm{d}\lambda) = \int_{\mathbb{R}} \frac{\pi_n(t;\mathrm{d}\lambda)}{z-t}\,\mathrm{d}\lambda(t). \tag{2.3.1}$$

(We omit the factor $1/(2\pi\mathrm{i})$ normally associated with Cauchy integrals, and for convenience also changed the sign.) The support interval $[a,b]$ of $\mathrm{d}\lambda$ is typically a finite, half-infinite, or doubly infinite interval. In the first two cases, (2.3.1) represents an analytic function in the connected domain $\mathbb{C}\backslash[a,b]$, in the last case two separate analytic functions, one in the upper half-plane and the other in the lower half-plane.

Cauchy integrals of orthogonal polynomials (also known as *functions of the second kind*) occur in many applications; for example, in the study of the Gauss quadrature error for analytic functions, where they appear as numerator in the kernel of the remainder term (Example 2.47), in modification algorithms involving division of a measure by a polynomial (Example 2.49 and §2.4.1), in the Stieltjes–Perron inversion formula recovering the measure of an orthogonal polynomial from its recurrence coefficients (Example 2.50), and in evaluating the Hilbert transform of a measure (Example 2.51). It is useful, therefore, to have reliable methods available for computing Cauchy integrals. The method we consider here is one that utilizes the basic three-term recurrence relation in the complex plane (cf. §1.3.5).

2.3.1 *Characterization in terms of minimal solutions*

The integral in (2.3.1) is nothing but the function $\rho_n(z)$ already introduced in (1.3.39),

$$(\mathcal{C}\pi_n)(z;\mathrm{d}\lambda) = \rho_n(z;\mathrm{d}\lambda), \quad n = 0,1,2,\ldots\ . \tag{2.3.2}$$

If, as in Theorem 1.43, we define

$$\rho_{-1}(z) = 1 \tag{2.3.3}$$

and assume that the moment problem for the measure $\mathrm{d}\lambda$ is determined, then from Corollary to Theorem 1.43 we know that (2.3.2), (2.3.3), when $z \in \mathbb{C}\backslash[a,b]$, is a minimal solution (cf. Definition 1.42) of the three-term recurrence relation

$$y_{k+1} = (z - \alpha_k)y_k - \beta_k y_{k-1}, \quad k = 0, 1, 2, \ldots, \tag{2.3.4}$$

where $\alpha_k = \alpha_k(\mathrm{d}\lambda)$, $\beta_k = \beta_k(\mathrm{d}\lambda)$. Moreover,

$$\frac{\rho_n(z)}{\rho_{n-1}(z)} = \frac{\beta_n}{z - \alpha_n -} \frac{\beta_{n+1}}{z - \alpha_{n+1} -} \frac{\beta_{n+2}}{z - \alpha_{n+2} -} \cdots, \quad n = 0, 1, 2, \ldots, \quad z \in \mathbb{C}\backslash[a, b]. \tag{2.3.5}$$

Computing $\rho_n(z)$ for $z \in \mathbb{C}\backslash[a, b]$ thus amounts to computing the minimal solution of (2.3.4) satisfying (2.3.3).

It is important to note that the "strength" of minimality of $\rho_n(z)$ weakens as z approaches the support interval $[a, b]$ of $\mathrm{d}\lambda$ and ceases altogether in the limit. If x is in the open interval (a, b), then (2.3.1) has to be interpreted as a Cauchy principal value integral,

$$\rho_n(x) = \int\!\!\!\!\!\!-_{\mathbb{R}} \frac{\pi_n(t; \mathrm{d}\lambda)}{x - t}\, \mathrm{d}\lambda(t); \tag{2.3.6}$$

it also satisfies the recurrence relation (2.3.4), but with initial values

$$\rho_{-1}(x) = 1, \quad \rho_0(x) = \int\!\!\!\!\!\!-_{\mathbb{R}} \frac{\mathrm{d}\lambda(t)}{x - t}. \tag{2.3.7}$$

The $\rho_n(x)$ can be computed from (2.3.4) (where $z = x$) in a stable manner by forward recursion. By Sokhotskyi's formulas (cf. Henrici (1986, Theorems 14.1a–c)) one has

$$\rho_n(x) = \frac{1}{2}\left(\lim_{z \downarrow x} \rho_n(z) + \lim_{z \uparrow x} \rho_n(z)\right), \tag{2.3.8}$$

where the two limits on the right are taken as z approaches x from above, resp. from below, the real axis. Since $z \uparrow x$ is the same as $\overline{z} \downarrow x$ and $\rho_n(\overline{z}) = \overline{\rho_n(z)}$, we can write (2.3.8) in the form

$$\rho_n(x) = \lim_{z \downarrow x} \mathrm{Re}\, \rho_n(z). \tag{2.3.9}$$

For each z, this requires only one evaluation of ρ_n.

2.3.2 *A continued fraction algorithm*

There are a number of algorithms available for computing minimal solutions of three-term recurrence relations (see, e.g. Wimp (1984)). In the case at hand, we have found most satisfactory an algorithm developed in Gautschi (1967a, §3), which is based on the continued fraction (2.3.5); see Gautschi (1981a, §5).

Suppose we wish to compute $\rho_n(z)$, $z \in \mathbb{C}\backslash[a, b]$, for $n = 0, 1, 2, \ldots, N$. (The value at $n = -1$ is known from (2.3.3).) Define

$$r_n = \frac{\rho_{n+1}(z)}{\rho_n(z)}, \quad n = -1, 0, 1, 2, \ldots, \tag{2.3.10}$$

and suppose for the moment that r_ν is known for some $\nu \geq N$. Then, by (2.3.5),

$$r_{n-1} = \frac{\beta_n}{z-\alpha_n-} \frac{\beta_{n+1}}{z-\alpha_{n+1}-} \frac{\beta_{n+2}}{z-\alpha_{n+2}-} \cdots, \quad n = 0, 1, 2, \ldots,$$

from which

$$r_{n-1} = \frac{\beta_n}{z-\alpha_n-r_n}, \quad n = \nu, \nu-1, \ldots, 0. \tag{2.3.11}$$

Since the initial value of the desired solution is $\rho_{-1}(z) = 1$, we now obtain from (2.3.10) that

$$\rho_{-1}(z) = 1, \quad \rho_n(z) = r_{n-1}\rho_{n-1}(z), \quad n = 0, 1, \ldots, N. \tag{2.3.12}$$

This completes the algorithm under the assumption made.

The actual algorithm follows this procedure very closely, except that in place of r_ν one uses zero. Thus, we define

$$r_\nu^{[\nu]} = 0, \quad r_{n-1}^{[\nu]} = \frac{\beta_n}{z-\alpha_n-} \frac{\beta_{n+1}}{z-\alpha_{n+1}-} \cdots \frac{\beta_\nu}{z-\alpha_\nu}, \tag{2.3.13}$$

and proceed according to

$$\begin{aligned} &r_\nu^{[\nu]} = 0, \quad r_{n-1}^{[\nu]} = \frac{\beta_n}{z-\alpha_n-r_n^{[\nu]}}, \quad n = \nu, \nu-1, \ldots, 0, \\ &\rho_{-1}^{[\nu]} = 1, \quad \rho_n^{[\nu]} = r_{n-1}^{[\nu]}\rho_{n-1}^{[\nu]}, \quad n = 0, 1, \ldots, N. \end{aligned} \tag{2.3.14}$$

It will presently be shown that for any fixed $n \geq 0$,

$$\lim_{\nu\to\infty} \rho_n^{[\nu]} = \rho_n(z). \tag{2.3.15}$$

Our algorithm consists in repeating (2.3.14) for a sequence of increasing values of ν until convergence in (2.3.15) is obtained for $n = 0, 1, \ldots, N$ to within a prescribed accuracy.

To convince ourselves of (2.3.15), we first provide the following alternative interpretation of (2.3.14). Let $\eta_k^{[\nu]}$ be the solution of the recurrence relation (2.3.4) defined by the starting values

$$\eta_\nu^{[\nu]} = 1, \quad \eta_{\nu+1}^{[\nu]} = 0. \tag{2.3.16}$$

The values of $\eta_k^{[\nu]}$ for $-1 \leq k \leq \nu-1$ may be obtained by applying (2.3.4) in the backward direction, starting at $k = \nu$. We then define

$$y_n^{[\nu]} := \frac{\rho_{-1}(z)}{\eta_{-1}^{[\nu]}} \eta_n^{[\nu]}, \quad -1 \leq n \leq N, \tag{2.3.17}$$

and will show that

$$y_n^{[\nu]} = \rho_n^{[\nu]}. \tag{2.3.18}$$

In this form, the algorithm is known as *Miller's algorithm*; it was proposed by J. C. P. Miller in 1952 in the context of computing spherical Bessel functions (British Association for the Advancement of Science, 1952, p. xvii).

Clearly, (2.3.18) holds when $n = -1$, since $y_{-1}^{[\nu]} = \rho_{-1}(z) = 1 = \rho_{-1}^{[\nu]}$. For $n > -1$, we note that

$$r_{n-1}^{[\nu]} = \frac{\eta_n^{[\nu]}}{\eta_{n-1}^{[\nu]}}, \quad 0 \le n \le \nu + 1.$$

Indeed, this is trivial for $n = \nu + 1$, and for $n \le \nu$ follows from the fact that the ratio on the right satisfies the same nonlinear recursion (2.3.11) satisfied by $r_{n-1}^{[\nu]}$. By (2.3.17), we have $y_n^{[\nu]}/y_{n-1}^{[\nu]} = \eta_n^{[\nu]}/\eta_{n-1}^{[\nu]}$; hence, $y_n^{[\nu]}/y_{n-1}^{[\nu]} = r_{n-1}^{[\nu]}$, $0 \le n \le N$. Thus, $y_n^{[\nu]}$ satisfies the same recursion as $\rho_n^{[\nu]}$ in (2.3.14) and has the same initial value 1, proving (2.3.18).

Now, let $\{y_n\} = \{y_n(z)\}$ be any solution of the recurrence relation (2.3.4) linearly independent of $\{\rho_n\} = \{\rho_n(z)\}$, so that by the minimality of $\{\rho_n\}$

$$\lim_{n\to\infty} \frac{\rho_n}{y_n} = 0.$$

Since $\{\eta_n^{[\nu]}\}$ is a solution of the same recurrence relation, it follows from the theory of linear difference equations that

$$\eta_n^{[\nu]} = a^{[\nu]}\rho_n + b^{[\nu]}y_n \tag{2.3.19}$$

for some constants $a^{[\nu]}$, $b^{[\nu]}$. In view of the two starting values (2.3.16), we have

$$\begin{aligned} a^{[\nu]}\rho_\nu + b^{[\nu]}y_\nu &= 1, \\ a^{[\nu]}\rho_{\nu+1} + b^{[\nu]}y_{\nu+1} &= 0, \end{aligned}$$

hence $b^{[\nu]} = -(\rho_{\nu+1}/y_{\nu+1})a^{[\nu]}$, so that

$$\eta_n^{[\nu]} = a^{[\nu]}\left(\rho_n - \frac{\rho_{\nu+1}}{y_{\nu+1}}\, y_n\right), \quad n = -1, 0, 1, 2, \dots .$$

Inserting this in (2.3.17) and noting (2.3.18) finally yields

$$\rho_n^{[\nu]} = \rho_n \frac{1 - \dfrac{\rho_{\nu+1}}{y_{\nu+1}}\dfrac{y_n}{\rho_n}}{1 - \dfrac{\rho_{\nu+1}}{\rho_{-1}y_{\nu+1}}\, y_{-1}}. \tag{2.3.20}$$

By the minimality of $\{\rho_n\}$, we have $\rho_{\nu+1}/y_{\nu+1} \to 0$ as $\nu \to \infty$, which proves (2.3.15).

The continued fraction algorithm based on (2.3.14) for computing $\rho_n(z)$, $0 \le n \le N$, is implemented in the `OPQ` routine `cauchy.m`. Testing for convergence in this routine is done on the quantities $r_{n-1}^{[\nu]}$, $n = 0, 1, \dots, N$, and only after convergence has occurred are $\rho_n(z)$ generated according to (2.3.12). The

routine, moreover, expects the user to provide a suitable starting value ν_0 for (2.3.14) to be employed with ν-values $\nu_0, \nu_0 + 5, \nu_0 + 10, \ldots$ until convergence. Some classical measures $\mathrm{d}\lambda$ allow realistic starting values ν_0 to be derived from asymptotic properties of the solutions of (2.3.4); see Gautschi (1981a, §5). They are implemented in the `OPQ` routines `nu0jac.m`, `nu0lag.m`, `nu0her.m` in the case of Jacobi, generalized Laguerre, and Hermite measures, respectively.

2.3.3 *Examples*

In our first example we return to the Gauss quadrature formula (1.4.7) and develop an alternative representation for the remainder term when the function to be integrated is analytic. The expression for the remainder given earlier in Corollary to Theorem 1.48 is of limited practical use since it requires knowledge of a high-order derivative of the integrand.

Example 2.47 *Remainder term of the Gauss quadrature formula* for analytic functions.

Theorem 2.48 *Let* $\mathrm{d}\lambda$ *be a measure supported on the finite interval* $[a, b]$ *and* $\mathcal{D} \subset \mathbb{C}$ *a domain in the complex plane containing* $[a, b]$ *in its interior. If* f *is analytic in* $\mathcal{D}$*, the Gauss quadrature remainder* R_n^G (cf. (1.4.7)) *can be expressed in the form*

$$R_n^G(f) = \frac{1}{2\pi \mathrm{i}} \oint_\Gamma K_n(z) f(z)\, \mathrm{d}z, \tag{2.3.21}$$

where Γ *is a simple closed curve in* $\mathcal{D}$ *encircling* $[a, b]$ *(in the positive sense) and* K_n*, the* kernel *of the remainder, is given by*

$$K_n(z) = K_n(z; \mathrm{d}\lambda) = \frac{\rho_n(z; \mathrm{d}\lambda)}{\pi_n(z; \mathrm{d}\lambda)}, \quad n = 0, 1, 2, \ldots . \tag{2.3.22}$$

Remark to Theorem 2.48 If $n = 0$, the quadrature sum is empty, and, therefore, $R_0^G(f) = \int_{\mathbb{R}} f(t)\, \mathrm{d}\lambda(t)$.

Proof Apply Cauchy's formula to f, both in the integral and the quadrature sum of (1.4.7), to obtain

$$\int_{\mathbb{R}} \frac{1}{2\pi \mathrm{i}} \oint_\Gamma \frac{f(z)\, \mathrm{d}z}{z - t}\, \mathrm{d}\lambda(t) = \sum_{\nu=1}^{n} \frac{\lambda_\nu^G}{2\pi \mathrm{i}} \oint_\Gamma \frac{f(z)}{z - \tau_\nu^G}\, \mathrm{d}z + R_n^G(f).$$

Interchanging the order of integration, one finds

$$R_n^G(f) = \frac{1}{2\pi \mathrm{i}} \oint_\Gamma K_n(z) f(z)\, \mathrm{d}z,$$

with K_n in the form

$$K_n(z) = \int_{\mathbb{R}} \frac{\mathrm{d}\lambda(t)}{z - t} - \sum_{\nu=1}^{n} \frac{\lambda_\nu^G}{z - \tau_\nu^G}, \quad n \geq 0. \tag{2.3.23}$$

By Theorem 1.47, the sum on the right equals $\sigma_n(z)/\pi_n(z)$, so that (2.3.22) follows from (2.3.23) and (1.3.40). □

The OPQ routine `kernel.m` evaluates $K_n(z)$, $n = 0, 1, \ldots, N$, from (2.3.22) in conjunction with the routine `cauchy.m`.

From (2.3.21) one obtains the simple error bound

$$|R_n^G(f)| \le \frac{\ell(\Gamma)}{2\pi} \max_{z\in\Gamma} |K_n(z; \mathrm{d}\lambda)| \cdot \max_{z\in\Gamma} |f(z)|, \tag{2.3.24}$$

where $\ell(\Gamma)$ is the length of the contour Γ, or else

$$|R_n^G(f)| \le \frac{1}{2\pi} \max_{z\in\Gamma} |K_n(z; \mathrm{d}\lambda)| \oint_\Gamma |f(z)||\,\mathrm{d}z|. \tag{2.3.25}$$

While the value of the error in (2.3.21) does not depend on the choice of the contour Γ, the bounds in (2.3.24) and (2.3.25) do. There are two classes of contours Γ often used in these bounds. Assuming $[a, b] = [-1, 1]$, they are the circles

$$C_r = \{z \in \mathbb{C} : \ |z| = r\}, \quad r > 1, \tag{2.3.26}$$

and confocal ellipses

$$\mathcal{E}_\rho = \{z \in \mathbb{C} : \ z = \tfrac{1}{2}(\rho \mathrm{e}^{\mathrm{i}\vartheta} + \rho^{-1}\mathrm{e}^{-\mathrm{i}\vartheta}), \ 0 \le \vartheta \le 2\pi\}, \quad \rho > 1, \tag{2.3.27}$$

with foci at ± 1 and sum of semiaxes equal to ρ. As $\rho \downarrow 1$, the ellipse $\mathcal{E}_\rho$ shrinks to the interval $[-1, 1]$, while with increasing ρ it becomes more and more circle-like. Poles of f that may be present in the vicinity of $[-1, 1]$ can thus be avoided by taking ρ sufficiently small. Circular contours are less flexible in this regard.

Problems of interest in connection with the bounds in (2.3.24) and (2.3.25) are (1) to locate and evaluate (or estimate) the maximum of the kernel K_n on $\Gamma = C_r$ resp. $\Gamma = \mathcal{E}_\rho$, and (2) to optimize the bounds over r resp. ρ.

For the classical Gauss–Legendre formula ($\mathrm{d}\lambda(t) = \mathrm{d}t$ on $[-1, 1]$), a contour map of $|K_{10}(z; \mathrm{d}t)|$, produced by the OPQ routine `Figure2_3.m`, is shown in Fig. 2.3. The contours are symmetric with respect to both axes, so that the map is shown only in the first quadrant of the complex plane. The curves correspond to the moduli $10^{-4}, 10^{-6}, 10^{-8}, \ldots, 10^{-16}$, as partially labeled in the figure.

The problem of computing recurrence coefficients for a modified measure—a measure multiplied by a rational function—will be solved in §2.4 by means of nonlinear recurrence algorithms. These, when the modification involves division by a polynomial, also require Cauchy integrals and hence the application of the continued fraction algorithm. Alternatively, as in Example 2.49, the use of appropriate modified moments and the modified Chebyshev algorithm (see §2.1.7) is another option.

Example 2.49 *Division of a measure by a polynomial.*

Let $\mathrm{d}\lambda$ be a positive measure on $\mathbb{R}$ and $q(t)$ a polynomial having constant sign as t varies on the support interval $[a, b]$ of $\mathrm{d}\lambda$. We wish to compute the recurrence coefficients $\hat{\alpha}_k$ and $\hat{\beta}_k$ for the modified measure $\mathrm{d}\hat{\lambda} = \mathrm{d}\lambda/q$. (When q is negative on $[a, b]$, the measure $\mathrm{d}\hat{\lambda}$ will be negative definite, hence $\hat{\beta}_0 < 0$.

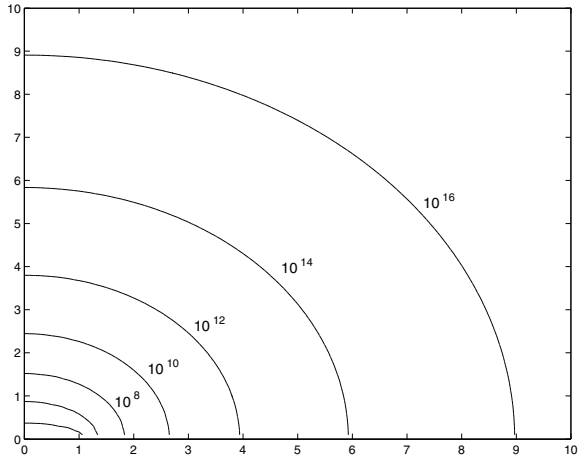

FIG. 2.3. Contour map of the kernel $K_{10}(z)$ for Gauss–Legendre quadrature.

One could avoid this by multiplying q by -1, but we will not bother doing this here.) It suffices to consider linear and quadratic divisors since algorithms that work for these can then be applied in succession after q has been factored into its linear and quadratic factors. Thus, we may assume that q is either $q(t) = t - x$ or $q(t) = (t-x)^2 + y^2$, $y > 0$, where in the first case $[a, b]$ is not all of $\mathbb{R}$ and x outside of $[a, b]$. The modified measure, therefore, is either

$$\mathrm{d}\hat{\lambda}(t) = \frac{\mathrm{d}\lambda(t)}{t-x}, \quad x \in \mathbb{R}\backslash[a,b], \tag{2.3.28}$$

or

$$\mathrm{d}\hat{\lambda}(t) = \frac{\mathrm{d}\lambda(t)}{(t-x)^2+y^2}, \quad x \in \mathbb{R},\ y > 0. \tag{2.3.29}$$

To compute $\hat{\alpha}_k, \hat{\beta}_k$, $k = 0, 1, \ldots, n$, we propose to use the modified Chebyshev algorithm, using the polynomials $\pi_k(\,\cdot\,; \mathrm{d}\lambda)$ to define the modified moments m_k (cf. (2.1.23)),

$$m_k = \int_{\mathbb{R}} \pi_k(t; \mathrm{d}\lambda)\, \mathrm{d}\hat{\lambda}(t), \quad k = 0, 1, \ldots, 2n-1. \tag{2.3.30}$$

In the case (2.3.28), this yields

$$m_k = \int_{\mathbb{R}} \frac{\pi_k(t; \mathrm{d}\lambda)}{t-x}\, \mathrm{d}\lambda(t) = -\rho_k(x), \tag{2.3.31}$$

where $\rho_k(x)$ is the Cauchy integral $(\mathcal{C}\pi_k)(x; \mathrm{d}\lambda)$ of (2.3.1). In the case (2.3.29), we let $z = x + \mathrm{i}y$ and write

$$\frac{1}{(x-t)^2+y^2} = -\frac{1}{2\mathrm{i}y}\left(\frac{1}{z-t} - \frac{1}{\overline{z}-t}\right)$$

to obtain

$$m_k = \int_{\mathbb{R}} \frac{\pi_k(t;\mathrm{d}\lambda)}{(x-t)^2+y^2}\,\mathrm{d}\lambda(t) = -\frac{\operatorname{Im}\rho_k(z)}{\operatorname{Im} z}\,. \tag{2.3.32}$$

In either case, the continued fraction algorithm of §2.3.2 can be applied to compute the modified moments in (2.3.30), which then can be employed by the modified Chebyshev algorithm to compute the recurrence coefficients $\hat{\alpha}_k$ and $\hat{\beta}_k$. This is implemented in the `OPQ` routines `gchri1.m` and `gchri2.m`. Numerical examples and comparisons with other (more efficient) modification algorithms will be given later in §2.4.6.

The case where $n = 0$ in (2.3.1) or (2.3.6) is not without interest, as the remaining two examples are to show.

Example 2.50 *Stieltjes–Perron inversion formula.*

Assume $\mathrm{d}\lambda(t) = w(t)\,\mathrm{d}t$ in (2.3.1) absolutely continuous, and suppose we know the recurrence coefficients α_k and β_k of $\mathrm{d}\lambda$. We may be asked to determine the support interval $[a,b]$ of $\mathrm{d}\lambda$ and to compute $w(x)$ for any $x \in (a,b)$. In a sense, this is the inverse of the main problem considered in this book. We will not consider here the first part of the problem—that of determining $[a,b]$. There is a detailed discussion of this in Chihara (1978, Chapter 4). A solution of the second part can be given in terms of the *Stieltjes–Perron formula* (cf. Henrici (1986, §14.6)), which in our notation asserts that

$$w(x) = -\frac{1}{\pi}\lim_{z\downarrow x}\operatorname{Im}\rho_0(z), \quad x \in (a,b). \tag{2.3.33}$$

To implement this computationally, put $z = x + \mathrm{i}y$ and let y approach 0 over a sequence of monotonically decreasing values $y = y_j$, $j = 1,2,\ldots$. If we denote $z_j = x + \mathrm{i}y_j$, $w_j = -\operatorname{Im}\rho_0(z_j)/\pi$, then $\lim_{j\to\infty} w_j = w(x)$. Each w_j can be computed by the continued fraction algorithm (2.3.14), where $z = z_j$ and $N = 0$, hence $\rho_0^{[\nu]} = r_{-1}^{[\nu]}$. Thus, only backward recursion is required in (2.3.14). It is in this part of the algorithm where the known recurrence coefficients α_k and β_k find their use. Since the minimality of $\{\rho_n(z_j)\}$ weakens with increasing j, larger and larger values of ν will be needed to achieve convergence in (2.3.15). Moreover, convergence of w_j to $w(x)$ as $j \to \infty$ may be quite slow, all of which suggests that the method as described may be impractical. This indeed is found to be true. Nevertheless, the method can be turned into a viable algorithm, at least for finite intervals $[a,b]$ and for accuracy requirements that are not too stringent, if the generation of the w_j is combined with a suitable convergence acceleration procedure. Specifically, we have chosen $y_j = 2^{-j}$, $j = 1,2,\ldots$, and applied to w_j, $j = 1,2,\ldots$, the well-known ε-algorithm (cf. Brezinski and Redivo Zaglia (1991, §2.3)).

The algorithm is embodied in the `OPQ` routine `SPHT.m`, with `iopt`=1, which for given $J \geq 1$ generates w_j, $j = 1,2,\ldots,J$, and applies on them the ε-algorithm. The latter is provided in the routine `epsalg.m`, a simple implementation of the "progressive form" of the ε-algorithm.

A feel for the method can be obtained by applying it to the recurrence coefficients of the Jacobi polynomials with parameters α and β and regenerating from them the Jacobi weight. We considered selected values of α and β in the region $-1 < \alpha \le \beta \le 1$ and selected x-values in $-1 < x < 1$, and computed w_j, $j = 1, 2, \ldots, J$, to a prescribed accuracy `eps0`. Among these, w_J is the most accurate approximation to $w(x)$; we want to observe how much the ε-algorithm can improve it. Using $J = 9$ and `eps0`$=10^{-6}$, we found that w_J approximates $w(x)$ generally to within an error of 10^{-3}, whereas the ε-algorithm was able, in general, to reduce the error to $10^{-5} - 10^{-6}$, but occasionally to an error as small as 10^{-9}. For x very close to the end points of $[-1, 1]$, the procedure becomes ineffective; see the `OPQ` routine `SPjac.m`.

A more interesting example is provided by the recurrence coefficients $\alpha_k = \alpha_k^{[1]}$, $\beta_k = \beta_k^{[1]}$ of the first numerator polynomials $\pi_k^{[1]}(\,\cdot\,; \mathrm{d}t)$ of the Legendre measure (cf. Definition 1.35), that is, $\alpha_k^{[1]} = \alpha_{k+1}^L$, $\beta_k^{[1]} = \beta_{k+1}^L$, $k = 0, 1, 2, \ldots$, where α_k^L and β_k^L are the ordinary Legendre coefficients. The corresponding measure is known to be $\mathrm{d}\lambda^{[1]}(t) = w^{[1]}(t)\,\mathrm{d}t$, where

$$w^{[1]}(t) = \frac{1}{[\ln(1+t)/(1-t)]^2 + \pi^2}\,, \quad -1 < t < 1$$

(cf. Example 1.37). For $\beta_0^{[1]}$ one must take the integral $\int_{-1}^{1} w^{[1]}(t)\,\mathrm{d}t$ (not β_1^L), which was found (numerically) to be 1/6. We applied `SPHT.m` with `iopt`=1 for $x = 0$ and $J = 9$, asking for an accuracy of `eps0`$=10^{-6}$ and limiting ν in (2.3.14) to $\nu \le$ `numax`=4000. (The actual value of ν that yielded convergence was found to be $\nu = 3895$.) We used the standard estimate `nu0`=.75×`numax`=3000. The results are displayed in the upper part of Table 2.20, which in the second column

Table 2.20 *Stieltjes–Perron inversion for the first numerator Legendre polynomials.*

j	err w_j	err ε_2	err ε_4	err ε_6	err ε_8
1	3.715(–2)	4.583(–3)	2.456(–5)	5.718(–8)	5.140(–8)
2	2.107(–2)	8.626(–4)	9.450(–7)	9.632(–9)	
3	1.118(–2)	1.865(–4)	1.148(–8)	1.147(–8)	
4	5.754(–3)	4.327(–5)	9.628(–9)		
5	2.918(–3)	1.042(–5)	3.435(–7)		
6	1.469(–3)	2.555(–6)			
7	7.370(–4)	8.330(–7)			
8	3.691(–4)				
9	1.847(–4)				

x	.2	.4	.6	.8	.9	.99
err w_9	1.859(–4)	1.898(–4)	1.995(–4)	2.294(–4)	2.858(–4)	1.005(–3)
err ε_8	9.197(–8)	1.108(–7)	6.150(–7)	5.965(–9)	5.315(–6)	7.315(–4)

shows the errors $|w_j - w(x)|$, $j = 1, 2, \ldots, J$, and in the subsequent columns the errors of the respective accelerated approximations produced by the ε-algorithm. As can be seen, the best of these, rather remarkably, is about 10^{-8}, which is smaller than the requested accuracy by two orders of magnitude. Similar results were obtained for other values of x, although the effectiveness of the procedure deteriorates as x approaches 1. This is shown in the lower part of Table 2.20, which displays $\operatorname{err} w_9$ and $\operatorname{err} \varepsilon_8$ for selected values of x. (For the corresponding negative values the results are the same by symmetry.) The computations are performed in the `OPQ` routine `Table2_20.m`.

Unfortunately, and not unexpectedly, the procedure has difficulty with unbounded intervals $[a, b]$ because of the exceedingly high values of ν required to achieve convergence in (2.3.15) when z approaches $[a, b]$. Even a sequence y_j converging to zero more slowly than 2^{-j} proved unsuccessful.

Example 2.51 *Hilbert transform of a measure.*

Given a measure $\mathrm{d}\lambda(t) = w(t)\,\mathrm{d}t$, its *Hilbert transform* is defined by

$$h(x) = (\mathcal{H}w)(x) := \int\!\!\!\!\!\!-_{\mathbb{R}} \frac{w(t)}{t - x}\,\mathrm{d}t, \quad a < x < b, \tag{2.3.34}$$

where $[a, b]$ is the support interval of $\mathrm{d}\lambda$. (We omit the factor $1/\pi$ normally associated with Hilbert transforms.) By (2.3.7), $h(x)$ is the same as $-\rho_0(x)$, and thus by (2.3.9),

$$h(x) = -\lim_{z \downarrow x} \operatorname{Re} \rho_0(z). \tag{2.3.35}$$

The same procedures as developed in Example 2.50 and implemented in `SPHT.m` are again applicable, the only difference being that in place of the imaginary part we now use the real part of $\rho_0(z)$. The Jacobi weight function $w(t) = (1 - t)^\alpha (1 + t)^\beta$ now presents a more interesting example since computing its Hilbert transform is a highly nontrivial task (cf., e.g. Gautschi and Wimp (1987)). We illustrate the procedure in the two cases $\alpha = \beta = -\frac{1}{2}$ and $\alpha = \beta = \frac{1}{2}$ (Chebyshev weight functions of the first and second kind). For these, the Hilbert transform is known explicitly: $h(x) = 0$ on $(-1, 1)$ in the former, and $h(x) = -\pi x$ on $(-1, 1)$ in the latter case. Table 2.21 shows the results for the same x-values as in the lower part of Table 2.20; the first two lines correspond to $\alpha = \beta = -\frac{1}{2}$, the next two lines to $\alpha = \beta = \frac{1}{2}$. See the `OPQ` routine `HTjac.m`.

2.4 Modification algorithms

Let $\mathrm{d}\lambda$ be a positive measure and

Table 2.21 *Hilbert transform of two Chebyshev measures.*

x	0.2	0.4	0.6	0.8	0.9	0.99
err w_9	1.305(–3)	3.188(–3)	7.190(–3)	2.272(–2)	6.666(–2)	2.114(0)
err ε_8	8.584(–7)	8.072(–7)	2.563(–7)	2.046(–6)	1.411(–3)	6.661(–1)
err w_9	1.252(–3)	2.678(–3)	4.602(–3)	8.181(–3)	1.267(–2)	4.286(–2)
err ε_8	2.285(–8)	1.043(–7)	2.438(–8)	3.858(–8)	9.364(–6)	3.187(–2)

$$u(t) = \pm \prod_{\lambda=1}^{\ell} (t - u_\lambda), \quad v(t) = \prod_{\mu=1}^{m} (t - v_\mu) \tag{2.4.1}$$

two real polynomials, relatively prime and not vanishing on the support $[a, b]$ of $\mathrm{d}\lambda$, the sign + or – in the former being chosen so that the ratio u/v is positive on $[a, b]$. We consider the *modified measure*

$$\mathrm{d}\hat{\lambda}(t) = \frac{u(t)}{v(t)}\,\mathrm{d}\lambda(t), \quad t \in [a, b], \tag{2.4.2}$$

and pose the problem of determining the recurrence coefficients of the modified measure, $\hat{\alpha}_k = \alpha_k(\mathrm{d}\hat{\lambda})$, $\hat{\beta}_k = \beta_k(\mathrm{d}\hat{\lambda})$, from those of the original measure, $\alpha_k = \alpha_k(\mathrm{d}\lambda)$, $\beta_k = \beta_k(\mathrm{d}\lambda)$. Methods that accomplish the passage from the αs and βs to the $\hat{\alpha}$s and $\hat{\beta}$s are called *modification algorithms*. They can be broken up into elementary steps, since the transition from $\mathrm{d}\lambda$ to $\mathrm{d}\hat{\lambda}$ need not be accomplished all at once but can be carried out one factor of u resp. v at a time. It suffices, therefore, to consider real linear factors $u(t) = t - x$ and real quadratic factors $u(t) = (t - x)^2 + y^2$ and analogous divisors. The respective modification algorithms are developed in §2.4.2–2.4.5. Examples are given in §2.4.6.

More classical is the related problem of expressing the orthogonal polynomials $\hat{\pi}_n = \pi_n(\,\cdot\,; \mathrm{d}\hat{\lambda})$ in terms of the $\pi_n = \pi_n(\,\cdot\,; \mathrm{d}\lambda)$. Solutions involving determinants will be briefly given in §2.4.1.

2.4.1 *Christoffel and generalized Christoffel theorems*

Christoffel was the first to express $u(\,\cdot\,)\pi(\,\cdot\,; \mathrm{d}\hat{\lambda})$ in the case $v(t) \equiv 1$ and $\mathrm{d}\lambda(t) = \mathrm{d}t$ in determinantal form as a linear combination of $\pi_n, \pi_{n+1}, \ldots, \pi_{n+\ell}$ (Christoffel (1858)). It was only 100 years later, in 1959, that the general case with $v(t) \not\equiv 1$ was solved by Uvarov (1959), (1969). For simplicity, we will assume that the zeros $u_1, u_2, \ldots, u_\ell$ of u and $v_1, v_2, \ldots, v_m$ of v are simple; extensions to multiple zeros are straightforward and involve derivatives of orthogonal polynomials. The results take on different forms depending on whether $m \le n$ or $m > n$.

Theorem 2.52 (Uvarov) *Let $m \le n$ and assume that u and v in (2.4.1) have only simple zeros. Then,*

$$u(t)\pi_n(t;\mathrm{d}\hat{\lambda}) = \text{const} \times \begin{vmatrix} \pi_{n-m}(t) & \cdots & \pi_{n-1}(t) & \pi_n(t) & \pi_{n+1}(t) & \cdots & \pi_{n+\ell}(t) \\ \pi_{n-m}(u_1) & \cdots & \pi_{n-1}(u_1) & \pi_n(u_1) & \pi_{n+1}(u_1) & \cdots & \pi_{n+\ell}(u_1) \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ \pi_{n-m}(u_\ell) & \cdots & \pi_{n-1}(u_\ell) & \pi_n(u_\ell) & \pi_{n+1}(u_\ell) & \cdots & \pi_{n+\ell}(u_\ell) \\ \rho_{n-m}(v_1) & \cdots & \rho_{n-1}(v_1) & \rho_n(v_1) & \rho_{n+1}(v_1) & \cdots & \rho_{n+\ell}(v_1) \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ \rho_{n-m}(v_m) & \cdots & \rho_{n-1}(v_m) & \rho_n(v_m) & \rho_{n+1}(v_m) & \cdots & \rho_{n+\ell}(v_m) \end{vmatrix}, \tag{2.4.3}$$

where

$$\rho_k(z) = \int_{\mathbb{R}} \frac{\pi_k(t;\mathrm{d}\lambda)}{z-t}\,\mathrm{d}\lambda(t), \quad k = 0, 1, 2, \dots\ . \tag{2.4.4}$$

Note that we have here another application of the Cauchy integrals of orthogonal polynomials.

The special case $m = 0$ is *Christoffel's theorem*, and (2.4.3) along with (2.4.5) may be referred to as *generalized Christoffel theorems*. If the new polynomial $\pi_n(\,\cdot\,;\mathrm{d}\hat{\lambda})$ is to be monic, the const in (2.4.3) has to be equal to the reciprocal of the (signed) cofactor of the element $\pi_{n+\ell}$ in the determinant of (2.4.3).

In the case $m > n$, a similar formula holds.

Theorem 2.53 (Uvarov) *Let $m > n$ and assume that u and v in (2.4.1) have only simple zeros. Then,*

$$u(t)\pi_n(t;\mathrm{d}\hat{\lambda}) = \text{const} \times \begin{vmatrix} 0 & 0 & 0 & \cdots & 0 & \pi_0(t) & \pi_1(t) & \cdots & \pi_{n+\ell}(t) \\ 0 & 0 & 0 & \cdots & 0 & \pi_0(u_1) & \pi_1(u_1) & \cdots & \pi_{n+\ell}(u_1) \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & 0 & \cdots & 0 & \pi_0(u_\ell) & \pi_1(u_\ell) & \cdots & \pi_{n+\ell}(u_\ell) \\ 1 & v_1 & v_1^2 & \cdots & v_1^{m-n-1} & \rho_0(v_1) & \rho_1(v_1) & \cdots & \rho_{n+\ell}(v_1) \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 1 & v_m & v_m^2 & \cdots & v_m^{m-n-1} & \rho_0(v_m) & \rho_1(v_m) & \cdots & \rho_{n+\ell}(v_m) \end{vmatrix}, \tag{2.4.5}$$

with $\rho_k(z)$ as defined in (2.4.4).

These results continue to hold for complex u_λ and v_μ if orthogonality is understood in the sense of formal orthogonality (cf. §1.6.1).

While Christoffel theorems are mathematically interesting and have found applications (in the asymptotic theory of orthogonal polynomials, for example), they are, in this generality, less useful for computational purposes. When m and n are small, however, the theorems will be used to derive modification algorithms.

2.4.2 *Linear factors*

Consider the modification

$$\mathrm{d}\hat{\lambda}(t) = (t-z)\,\mathrm{d}\lambda(t), \quad z \in \mathbb{C}\backslash[a,b]. \tag{2.4.6}$$

Here, $m = 0$, $\ell = 1$, and the monic polynomial $\hat{\pi}_n(\,\cdot\,) = \pi_n(\,\cdot\,;\mathrm{d}\hat{\lambda})$, by (2.4.3), is given by

$$(t-z)\hat{\pi}_n(t) = \frac{\begin{vmatrix} \pi_n(t) & \pi_{n+1}(t) \\ \pi_n(z) & \pi_{n+1}(z) \end{vmatrix}}{-\pi_n(z)} = \pi_{n+1}(t) - \frac{\pi_{n+1}(z)}{\pi_n(z)}\,\pi_n(t),$$

that is, $\hat{\pi}_n$ is the kernel polynomial of (1.6.5), in agreement with Theorem 1.55. In this and the following subsection, we shall use the notation

$$r_n = r_n(z) = \frac{\pi_{n+1}(z)}{\pi_n(z)}, \quad n = 0, 1, 2, \ldots, \tag{2.4.7}$$

which is well defined since z is outside the support interval of $\mathrm{d}\lambda$. Thus,

$$(t-z)\hat{\pi}_n(t) = \pi_{n+1}(t) - r_n\pi_n(t). \tag{2.4.8}$$

To obtain the connection between the new recurrence coefficients $\hat{\alpha}_k$, $\hat{\beta}_k$ for $\{\hat{\pi}_n\}$ and the old ones, α_k, β_k for $\{\pi_n\}$, we write $(t-z)t\hat{\pi}_k(t)$ in two different ways. First, we use the three-term recurrence relation for π_k in (2.4.8) to write

$$\begin{aligned}(t-z)t\hat{\pi}_k(t) &= t\pi_{k+1}(t) - r_k \cdot t\pi_k(t) \\ &= \pi_{k+2}(t) + \alpha_{k+1}\pi_{k+1}(t) + \beta_{k+1}\pi_k(t) - r_k[\pi_{k+1}(t) + \alpha_k\pi_k(t) + \beta_k\pi_{k-1}(t)] \\ &= \pi_{k+2}(t) + (\alpha_{k+1} - r_k)\pi_{k+1}(t) + (\beta_{k+1} - r_k\alpha_k)\pi_k(t) - r_k\beta_k\pi_{k-1}(t),\end{aligned} \tag{2.4.9}$$

and then use the three-term recurrence relation for $\hat{\pi}_k$ in combination with (2.4.8) to write

$$\begin{aligned}(t-z)t\hat{\pi}_k(t) &= (t-z)[\hat{\pi}_{k+1}(t) + \hat{\alpha}_k\hat{\pi}_k(t) + \hat{\beta}_k\hat{\pi}_{k-1}(t)] \\ &= \pi_{k+2}(t) - r_{k+1}\pi_{k+1}(t) + \hat{\alpha}_k[\pi_{k+1}(t) - r_k\pi_k(t)] + \hat{\beta}_k[\pi_k(t) - r_{k-1}\pi_{k-1}(t)] \\ &= \pi_{k+2}(t) + (\hat{\alpha}_k - r_{k+1})\pi_{k+1}(t) + (\hat{\beta}_k - r_k\hat{\alpha}_k)\pi_k(t) - r_{k-1}\hat{\beta}_k\pi_{k-1}(t).\end{aligned} \tag{2.4.10}$$

Comparing the coefficients in these two identities then yields

$$\begin{aligned}\hat{\alpha}_k - r_{k+1} &= \alpha_{k+1} - r_k, \\ \hat{\beta}_k - r_k\hat{\alpha}_k &= \beta_{k+1} - r_k\alpha_k, \\ r_{k-1}\hat{\beta}_k &= r_k\beta_k,\end{aligned}$$

and thus, from the first and third relations,

$$\hat{\alpha}_k = \alpha_{k+1} + r_{k+1} - r_k, \quad k \geq 0,$$
$$\hat{\beta}_k = r_k \beta_k / r_{k-1}, \quad k \geq 1.$$

The middle relation is automatically satisfied, as can be verified by expressing $\hat{\beta}_k$ and $\hat{\alpha}_k$ in terms of β_k and α_k, and using the relation

$$r_{k+1} = z - \alpha_{k+1} - \beta_{k+1}/r_k, \tag{2.4.11}$$

which follows from the recurrence relation for $\{\pi_k\}$. The constant $\hat{\beta}_0$, in line with our convention (1.3.6), should be defined by

$$\int_{\mathbb{R}} \mathrm{d}\hat{\lambda}(t) = \int_{\mathbb{R}} (t-z)\,\mathrm{d}\lambda(t) = \int_{\mathbb{R}} (t - \alpha_0 + \alpha_0 - z)\,\mathrm{d}\lambda(t)$$
$$= \int_{\mathbb{R}} \pi_1(t)\,\mathrm{d}\lambda(t) + (\alpha_0 - z)\int_{\mathbb{R}} \mathrm{d}\lambda(t),$$

hence, since the first integral on the right vanishes by orthogonality,

$$\hat{\beta}_0 = (\alpha_0 - z)\beta_0.$$

We thus arrive at the following algorithm.

Algorithm 2.5 (Modification by a linear factor)

Initialization:

$$r_0 = z - \alpha_0, \quad r_1 = z - \alpha_1 - \beta_1/r_0,$$
$$\hat{\alpha}_0 = \alpha_1 + r_1 - r_0, \quad \hat{\beta}_0 = -r_0\beta_0. \tag{2.4.12}$$

Continuation (if $n > 1$): for $k = 1, 2, \ldots, n-1$ do

$$r_{k+1} = z - \alpha_{k+1} - \beta_{k+1}/r_k,$$
$$\hat{\alpha}_k = \alpha_{k+1} + r_{k+1} - r_k, \tag{2.4.13}$$
$$\hat{\beta}_k = \beta_k r_k / r_{k-1}.$$

Note that the algorithm requires α_n, β_n in addition to the α_k, β_k for $k \leq n-1$. Algorithm 2.5 is implemented in the `OPQ` routine `chri1.m`.

2.4.3 *Quadratic factors*

The modified measure to be considered here is

$$\mathrm{d}\hat{\lambda}(t) = (t-z)(t-\overline{z})\,\mathrm{d}\lambda(t) = \big((t-x)^2 + y^2\big)\,\mathrm{d}\lambda(t), \tag{2.4.14}$$

where $z = x + \mathrm{i}y$, $x \in \mathbb{R}$, $y > 0$. We are now in the case $m = 0$, $\ell = 2$ of (2.4.3), where $u_1 = z$ and $u_2 = \overline{z}$, and consequently

$$(t-z)(t-\overline{z})\hat{\pi}_n(t) = \frac{\begin{vmatrix} \pi_n(t) & \pi_{n+1}(t) & \pi_{n+2}(t) \\ \pi_n(z) & \pi_{n+1}(z) & \pi_{n+2}(z) \\ \pi_n(\overline{z}) & \pi_{n+1}(\overline{z}) & \pi_{n+2}(\overline{z}) \end{vmatrix}}{\begin{vmatrix} \pi_n(z) & \pi_{n+1}(z) \\ \pi_n(\overline{z}) & \pi_{n+1}(\overline{z}) \end{vmatrix}}.$$

An elementary computation will show that

$$(t-z)(t-\overline{z})\hat{\pi}_n(t) = \pi_{n+2} + s_n\pi_{n+1} + t_n\pi_n(t), \tag{2.4.15}$$

where

$$s_n = -\left(r'_{n+1} + \frac{r''_{n+1}}{r''_n}\, r'_n\right), \quad t_n = \frac{r''_{n+1}}{r''_n}\,|r_n|^2.$$

Here, the notation

$$r'_n = \operatorname{Re} r_n(z),\ r''_n = \operatorname{Im} r_n(z),\ |r_n|^2 = |r_n(z)|^2, \quad n = 0, 1, 2, \ldots,$$

is used, where $r_n(z)$ continues to be the quantity defined in (2.4.7). To the identity (2.4.15) we now apply the same procedure that was used in (2.4.8)–(2.4.10), expanding $(t-z)(t-\overline{z})\cdot t\hat{\pi}_k(t)$ in two different ways into a linear combination of the five orthogonal polynomials $\pi_{k+3}, \pi_{k+2}, \ldots, \pi_{k-1}$. Comparison of the respective coefficients yields five equations relating the new recurrence coefficients to the old ones. The first and last of these equations are, respectively,

$$\begin{aligned} s_{k+1} + \hat{\alpha}_k &= s_k + \alpha_{k+2}, \quad k \geq 0, \\ t_{k-1}\hat{\beta}_k &= t_k\beta_k, \quad k \geq 1. \end{aligned}$$

For $\hat{\beta}_0$, we have

$$\begin{aligned} \hat{\beta}_0 &= \int_{\mathbb{R}} \left((t-x)^2 + y^2\right) \mathrm{d}\lambda(t) = \int_{\mathbb{R}} \left((t-\alpha_0+\alpha_0-x)^2 + y^2\right) \mathrm{d}\lambda(t) \\ &= \int_{\mathbb{R}} \left((t-\alpha_0)^2 + (\alpha_0-x)^2 + y^2\right) \mathrm{d}\lambda(t), \end{aligned}$$

where $\int_{\mathbb{R}} (t-\alpha_0)\,\mathrm{d}\lambda(t) = \int_{\mathbb{R}} \pi_1(t)\,\mathrm{d}\lambda(t) = 0$ has been used in the last equality. Furthermore (cf. (1.3.7)),

$$\int_{\mathbb{R}} (t-\alpha_0)^2\,\mathrm{d}\lambda(t) = \|\pi_1\|^2 = \beta_0\beta_1,$$

so that

$$\hat{\beta}_0 = \beta_0(\beta_1 + (\alpha_0 - x)^2 + y^2).$$

Making use of (2.4.11) again, we are led to the following algorithm.

Algorithm 2.6 (Modification by a quadratic factor)
Initialization:

$$\begin{aligned} &r_0 = z - \alpha_0, \quad r_1 = z - \alpha_1 - \beta_1/r_0, \quad r_2 = z - \alpha_2 - \beta_2/r_1, \\ &\hat{\alpha}_0 = \alpha_2 + r_2' + \frac{r_2''}{r_1''}\, r_1' - \left(r_1' + \frac{r_1''}{r_0''}\, r_0' \right), \\ &\hat{\beta}_0 = \beta_0(\beta_1 + |r_0|^2). \end{aligned} \tag{2.4.16}$$

Continuation (if $n > 1$): for $k = 1, 2, \ldots, n-1$ do

$$\begin{aligned} &r_{k+2} = z - \alpha_{k+2} - \beta_{k+2}/r_{k+1}, \\ &\hat{\alpha}_k = \alpha_{k+2} + r_{k+2}' + \frac{r_{k+2}''}{r_{k+1}''}\, r_{k+1}' - \left(r_{k+1}' + \frac{r_{k+1}''}{r_k''}\, r_k' \right), \\ &\hat{\beta}_k = \beta_k \frac{r_{k+1}'' r_{k-1}''}{[r_k'']^2} \left| \frac{r_k}{r_{k-1}} \right|^2. \end{aligned} \tag{2.4.17}$$

Here, we need α_k, β_k for $k \le n+1$. Algorithm 2.6 is implemented in the `OPQ` routine `chri2.m`.

In the special case where $\mathrm{d}\lambda$ is a symmetric measure (hence $\alpha_k = 0$ for all k) and $x = 0$, that is, for

$$\mathrm{d}\hat{\lambda}(t) = (t^2 + y^2)\, \mathrm{d}\lambda(t), \quad \mathrm{d}\lambda \text{ symmetric},$$

Algorithm 2.6 simplifies since all r_k are purely imaginary.

Algorithm 2.7 (Modification by a simplified symmetric quadratic factor)
Initialization:

$$\begin{aligned} &r_0'' = y, \quad r_1'' = y + \beta_1/y, \quad r_2'' = y + \beta_2/r_1'', \\ &\hat{\alpha}_0 = 0, \quad \hat{\beta}_0 = \beta_0(\beta_1 + y^2). \end{aligned} \tag{2.4.18}$$

Continuation (if $n > 1$): for $k = 1, 2, \ldots, n-1$ do

$$\begin{aligned} &r_{k+2}'' = y + \beta_{k+2}/r_{k+1}'', \\ &\hat{\alpha}_k = 0, \quad \hat{\beta}_k = \beta_k r_{k+1}''/r_{k-1}''. \end{aligned} \tag{2.4.19}$$

Algorithm 2.7 is implemented in the `OPQ` routine `chri3.m`. Algorithms 2.6 and 2.7 both appear to be numerically stable.

Another quadratic factor of interest is

$$\mathrm{d}\hat{\lambda}(t) = (t - x)^2\, \mathrm{d}\lambda(t), \quad x \in \mathbb{R}, \tag{2.4.20}$$

which still produces a nonnegative definite measure $\mathrm{d}\hat{\lambda}$ but one that will vanish inside the support $[a, b]$ of $\mathrm{d}\lambda$ if x is in (a, b). In this case, one could be tempted

to apply the algorithm for linear factors twice in succession, with the same value of x. But that could be risky since the underlying assumption $\pi_n(x; \mathrm{d}\lambda) \neq 0$, all n, may no longer be true. It is possible, however, to solve the problem by techniques of numerical linear algebra (cf. Gautschi (2002, §3.3)): *apply one step of the QR algorithm with shift x to the Jacobi matrix $\boldsymbol{J}_{n+2}(\mathrm{d}\lambda)$ of order $n+2$* (cf. (1.3.15)) *and discard the last two rows and columns of the resulting matrix to obtain $\boldsymbol{J}_n(\mathrm{d}\hat{\lambda})$.* This is implemented in the `OPQ` routine `chri7.m`.

2.4.4 *Linear divisors*

Let

$$\mathrm{d}\hat{\lambda}(t) = \frac{\mathrm{d}\lambda(t)}{t-z}, \quad z \in \mathbb{C}\backslash[a,b], \tag{2.4.21}$$

where $[a,b]$ is the support interval of $\mathrm{d}\lambda$. We are in the case $\ell = 0$, $m = 1$, $v_1 = z$ of Theorem 2.52, and therefore, letting $\hat{\pi}_n(\,\cdot\,) = \pi_n(\,\cdot\,; \mathrm{d}\hat{\lambda})$,

$$\hat{\pi}_n(t) = \frac{\begin{vmatrix} \pi_{n-1}(t) & \pi_n(t) \\ \rho_{n-1}(z) & \rho_n(z) \end{vmatrix}}{-\rho_{n-1}(z)} = \pi_n(t) - \frac{\rho_n(z)}{\rho_{n-1}(z)}\,\pi_{n-1}(t), \quad n \geq 1.$$

In analogy to (2.4.7), we now redefine r_n to be

$$r_n = r_n(z) = \frac{\rho_{n+1}(z)}{\rho_n(z)}, \quad n = -1, 0, 1, 2, \ldots; \quad \rho_{-1}(z) = 1, \tag{2.4.22}$$

where the last relation is consistent with (2.3.3). Thus,

$$\hat{\pi}_n(t) = \pi_n(t) - r_{n-1}\pi_{n-1}(t), \quad n = 1, 2, \ldots. \tag{2.4.23}$$

Expressing $t\hat{\pi}_k(t)$, as in §2.4.2–2.4.3, in two different ways as a linear combination of $\pi_{k+1}, \pi_k, \pi_{k-1}$, and π_{k-2}, and comparing coefficients, yields for $k \geq 2$

$$\begin{aligned} \hat{\alpha}_k &= \alpha_k + r_k - r_{k-1}, \\ \hat{\beta}_k &= \beta_{k-1} r_{k-1}/r_{k-2}. \end{aligned} \tag{2.4.24}$$

The same argument confirms the validity of the first relation in (2.4.24) for $k = 1$, and for $k = 0$ it gives

$$\hat{\alpha}_0 = \alpha_0 + r_0.$$

For $\hat{\beta}_1$, however, the procedure yields

$$\hat{\beta}_1 = \beta_1 + r_0(\hat{\alpha}_1 - \alpha_0).$$

From the discussion in §2.3.1, we recall that

$$\rho_{k+1}(z) = (z - \alpha_k)\rho_k(z) - \beta_k \rho_{k-1}(z), \quad k = 0, 1, 2, \ldots,$$

hence

$$\begin{aligned} r_k &= z - \alpha_k - \beta_k / r_{k-1}, \quad k = 0, 1, 2, \ldots, \\ r_{-1} &= \rho_0(z). \end{aligned} \tag{2.4.25}$$

In particular,

$$r_0 = z - \alpha_0 - \beta_0/\rho_0, \quad r_1 = z - \alpha_1 - \beta_1/r_0.$$

Inserting the second relation in

$$\hat{\beta}_1 = \beta_1 + r_0(\alpha_1 + r_1 - r_0 - \alpha_0),$$

and then making use of the first, yields $\hat{\beta}_1 = \beta_0 r_0/\rho_0$, which is the second relation in (2.4.24) for $k = 1$. Finally, by convention,

$$\hat{\beta}_0 = \int_{\mathbb{R}} \mathrm{d}\hat{\lambda}(t) = \int_{\mathbb{R}} \frac{\mathrm{d}\lambda(t)}{t - z} = -\rho_0(z).$$

In summary, then, we have the following algorithm.

Algorithm 2.8 (Modification by a linear divisor)

Initialization:

$$\hat{\alpha}_0 = \alpha_0 + r_0, \quad \hat{\beta}_0 = -\rho_0(z). \tag{2.4.26}$$

Continuation (if $n > 1$): for $k = 1, 2, \ldots, n-1$ do

$$\begin{aligned} \hat{\alpha}_k &= \alpha_k + r_k - r_{k-1}, \\ \hat{\beta}_k &= \beta_{k-1} r_{k-1} / r_{k-2}. \end{aligned} \tag{2.4.27}$$

In contrast to Algorithm 2.5, no coefficients α_k, β_k beyond $k \leq n-1$ are needed, in fact not even β_{n-1}.

It remains to discuss the computation of the quantities r_k in Algorithm 2.8. Since they are ratios ρ_{k+1}/ρ_k of the minimal solution $\{\rho_k\}$ of the basic three-term recurrence relation (cf. Theorem 1.43), they can be computed by the continued fraction algorithm of §2.3.2. As a matter of fact, they are simply the limits, as $\nu \to \infty$, of the quantities $r_k^{[\nu]}$ in (2.3.14) and are furnished in one of the output arrays of the routine `cauchy.m`. Moreover, $\rho_0 = r_{-1}$ is also produced by the continued fraction algorithm.

As z approaches the support interval $[a, b]$, minimality of $\{\rho_k\}$ weakens, and convergence of the continued fraction algorithm slows down. For z very close to the support interval and n not too large, on the other hand, we can safely generate the r_k by forward recursion as in (2.4.25). This, however, requires knowledge of $\rho_0(z)$. The routine `chri4.m`, which implements Algorithm 2.8, provides both options: with input parameter `iopt`=1 it uses the continued fraction algorithm, otherwise forward recursion.

2.4.5 *Quadratic divisors*

We now consider

$$\mathrm{d}\hat{\lambda}(t) = \frac{\mathrm{d}\lambda(t)}{(t-z)(t-\overline{z})} = \frac{\mathrm{d}\lambda(t)}{(t-x)^2+y^2}\,, \quad z = x+\mathrm{i}y,\ x\in\mathbb{R},\ y>0. \quad (2.4.28)$$

We begin by observing that

$$\hat{\alpha}_0 = \frac{\displaystyle\int_{\mathbb{R}} t\mathrm{d}\lambda(t)/|t-z|^2}{\displaystyle\int_{\mathbb{R}} \mathrm{d}\lambda(t)/|t-z|^2} = x + y\,\frac{\operatorname{Re}\rho_0(z)}{\operatorname{Im}\rho_0(z)}\,, \quad \hat{\beta}_0 = -\frac{1}{y}\operatorname{Im}\rho_0(z),$$

where $\rho_0(z)$ is the Cauchy integral (2.4.4) for $k=0$. We are in the case $\ell=0$, $m=2$ of the generalized Christoffel theorems (2.4.3) and (2.4.5), which give, for $\hat{\pi}_n(\,\cdot\,) = \pi_n(\,\cdot\,;\mathrm{d}\hat{\lambda})$,

$$\hat{\pi}_n(t) = \frac{\begin{vmatrix} \pi_{n-2}(t) & \pi_{n-1}(t) & \pi_n(t) \\ \rho_{n-2}(z) & \rho_{n-1}(z) & \rho_n(z) \\ \rho_{n-2}(\overline{z}) & \rho_{n-1}(\overline{z}) & \rho_n(\overline{z}) \end{vmatrix}}{\begin{vmatrix} \rho_{n-2}(z) & \rho_{n-1}(z) \\ \rho_{n-2}(\overline{z}) & \rho_{n-1}(\overline{z}) \end{vmatrix}},\ n\ge 2; \quad \hat{\pi}_1(t) = \frac{\begin{vmatrix} 0 & \pi_0(t) & \pi_1(t) \\ 1 & \rho_0(z) & \rho_1(z) \\ 1 & \rho_0(\overline{z}) & \rho_1(\overline{z}) \end{vmatrix}}{\begin{vmatrix} 1 & \rho_0(z) \\ 1 & \rho_0(\overline{z}) \end{vmatrix}}. \quad (2.4.29)$$

We continue to use the notation

$$r_n(z) = r_n' + \mathrm{i}r_n'', \quad \rho_n(z) = \rho_n' + \mathrm{i}\rho_n'', \quad |r_n(z)|^2 = |r_n|^2, \quad |\rho_n(z)|^2 = |\rho_n|^2.$$

Lemma 2.54 *There holds*

$$\hat{\pi}_n(t) = \pi_n(t) + s_n\pi_{n-1}(t) + t_n\pi_{n-2}(t), \quad n\ge 1, \quad (2.4.30)$$

where

$$s_n = -\left(r_{n-1}' + \frac{r_{n-1}''}{r_{n-2}''}\,r_{n-2}'\right),\ n\ge 1; \quad t_n = \frac{r_{n-1}''}{r_{n-2}''}\,|r_{n-2}|^2,\ n\ge 2, \quad (2.4.31)$$

and r_n is given by (2.4.22).

Proof Let first $n\ge 2$. Then, by the first of (2.4.29),

$$s_n = -\frac{\rho_{n-2}(z)\rho_n(\overline{z}) - \rho_{n-2}(\overline{z})\rho_n(z)}{\rho_{n-2}(z)\rho_{n-1}(\overline{z}) - \rho_{n-2}(\overline{z})\rho_{n-1}(z)}\,.$$

Dividing the numerator and the denominator by $\rho_{n-2}(z)\rho_{n-2}(\overline{z})$ yields

$$s_n = -\frac{r_{n-1}(z)r_{n-2}(z) - r_{n-1}(\overline{z})r_{n-2}(\overline{z})}{r_{n-2}(z) - r_{n-2}(\overline{z})} = -\frac{\operatorname{Im}\left[r_{n-1}(z)r_{n-2}(z)\right]}{\operatorname{Im} r_{n-2}(z)}\,,$$

from which the first relation in (2.4.31) follows for $n \geq 2$. Similarly,

$$t_n = \frac{\rho_{n-1}(z)\rho_n(\overline{z}) - \rho_{n-1}(\overline{z})\rho_n(z)}{\rho_{n-2}(z)\rho_{n-1}(\overline{z}) - \rho_{n-2}(\overline{z})\rho_{n-1}(z)}$$
$$= \frac{r_{n-1}(z) - r_{n-1}(\overline{z})}{r_{n-2}(z) - r_{n-2}(\overline{z})}\,|r_{n-2}(z)|^2 = \frac{\operatorname{Im} r_{n-1}(z)}{\operatorname{Im} r_{n-2}(z)}\,|r_{n-2}(z)|^2,$$

which is the second relation in (2.4.31).

It remains to prove the assertion for s_1. Here, we use the second formula in (2.4.29),

$$\hat{\pi}_1(t) = \pi_1(t) + s_1\pi_0(t),$$

and find

$$s_1 = -\frac{\rho_1(z) - \rho_1(\overline{z})}{\rho_0(z) - \rho_0(\overline{z})} = -\frac{r_0(z)\rho_0(z) - r_0(\overline{z})\rho_0(\overline{z})}{\rho_0(z) - \rho_0(\overline{z})} = -\frac{\operatorname{Im}\left[r_0(z)\rho_0(z)\right]}{\operatorname{Im}\rho_0(z)},$$

which is (2.4.31) for $n = 1$, recalling that $r_{-1}(z) = \rho_0(z)$. □

We now use the procedure, already applied repeatedly in §2.4.2–2.4.4, of expressing $t\hat{\pi}_k(t)$ in two different ways as linear combinations of the original polynomials $\pi_{k+1}, \pi_k, \ldots$, and comparing the corresponding coefficients. With $\hat{\pi}_k$ given in (2.4.30) and (2.4.31), this results in

$$\hat{\alpha}_k = \alpha_k - s_{k+1} + s_k, \quad \hat{\beta}_k = \beta_{k-2}\,t_k/t_{k-1} \quad \text{for } k \geq 3,$$
$$\hat{\alpha}_2 = \alpha_2 - s_3 + s_2, \quad \hat{\beta}_2 = \beta_2 + s_2(\alpha_1 - \hat{\alpha}_2) - t_3 + t_2 \quad \text{for } k = 2,$$

and

$$\hat{\alpha}_1 = \alpha_1 - s_2 + s_1, \quad \hat{\beta}_1 = \beta_1 + s_1(\alpha_0 - \hat{\alpha}_1) - t_2 \quad \text{for } k = 1.$$

We have obtained the following algorithm.

Algorithm 2.9 (Modification by a quadratic divisor)
Initialization:

$$\begin{aligned}
&\hat{\alpha}_0 = x + \rho_0' y/\rho_0'', \quad \hat{\beta}_0 = -\rho_0''/y,\\
&\hat{\alpha}_1 = \alpha_1 - s_2 + s_1, \quad \hat{\beta}_1 = \beta_1 + s_1(\alpha_0 - \hat{\alpha}_1) - t_2,\\
&\hat{\alpha}_2 = \alpha_2 - s_3 + s_2, \quad \hat{\beta}_2 = \beta_2 + s_2(\alpha_1 - \hat{\alpha}_2) - t_3 + t_2.
\end{aligned} \tag{2.4.32}$$

Continuation (if $n > 3$): for $k = 3, 4, \ldots, n-1$ do

$$\hat{\alpha}_k = \alpha_k - s_{k+1} + s_k, \quad \hat{\beta}_k = \beta_{k-2}\,t_k/t_{k-1}, \tag{2.4.33}$$

where the s_n and t_n are as defined in (2.4.31).

Algorithm 2.9 is implemented in the `OPQ` routine `chri5.m`. Like the routine `chri4.m`, it provides for two options, as explained in the last paragraph of §2.4.4.

Substantial simplifications occur if $\mathrm{d}\lambda$ is symmetric and $x = 0$, that is, in the case

$$\mathrm{d}\hat{\lambda}(t) = \frac{\mathrm{d}\lambda(t)}{t^2 + y^2}, \quad \mathrm{d}\lambda \text{ symmetric}, \ y > 0.$$

Then, $\alpha_k = \hat{\alpha}_k = 0$ for all k, and Algorithm 2.9 becomes

Algorithm 2.10 (Modification by a simplified symmetric quadratic divisor)
Initialization:

$$\begin{aligned} &\hat{\alpha}_0 = 0, \quad \hat{\beta}_0 = -\rho_0''/y, \\ &\hat{\alpha}_1 = 0, \quad \hat{\beta}_1 = \beta_1 - t_2, \\ &\hat{\alpha}_2 = 0, \quad \hat{\beta}_2 = \beta_2 - t_3 + t_2. \end{aligned} \tag{2.4.34}$$

Continuation (if $n > 3$): for $k = 3, 4, \ldots, n-1$ do

$$\hat{\alpha}_k = 0, \quad \hat{\beta}_k = \beta_{k-2}\, t_k / t_{k-1}, \tag{2.4.35}$$

where the t_n are as defined in (2.4.31).

Algorithm 2.10 is implemented in the `OPQ` routine `chri6.m`.

In quadrature problems that involve a pair of poles located symmetrically with respect to the origin just barely outside the (symmetric) interval $[a, b]$ of integration (cf. §3.1.4), modification by a special quadratic divisor,

$$\mathrm{d}\hat{\lambda}(t) = \frac{\mathrm{d}\lambda(t)}{t^2 - x^2}, \quad x \in \mathbb{R}\backslash[a, b], \tag{2.4.36}$$

is of interest. This can be treated exactly as before by replacing z by x and $\overline{z}$ by $-x$. It is convenient to write

$$\rho_n(x) = \rho_n^+, \quad \rho_n(-x) = \rho_n^- \quad \text{and} \quad r_n(x) = r_n^+, \quad r_n(-x) = r_n^-.$$

A simple computation then shows that

$$\hat{\alpha}_0 = x\, \frac{\rho_0^+ + \rho_0^-}{\rho_0^+ - \rho_0^-}, \quad \hat{\beta}_0 = -\frac{1}{2x}\,(\rho_0^+ - \rho_0^-),$$

and Lemma 2.54 becomes

Lemma 2.55 *For $\hat{\pi}_n(\,\cdot\,) = \pi_n(\,\cdot\,; \mathrm{d}\hat{\lambda})$, with $\mathrm{d}\hat{\lambda}$ given by (2.4.36), there holds*

$$\hat{\pi}_n(t) = \pi_n + s_n \pi_{n-1} + t_n \pi_{n-2}(t), \quad n \geq 1, \tag{2.4.37}$$

where

$$s_n = -\frac{\dfrac{r_{n-1}^-}{r_{n-2}^+} - \dfrac{r_{n-1}^+}{r_{n-2}^-}}{\dfrac{1}{r_{n-2}^+} - \dfrac{1}{r_{n-2}^-}}, \quad n \geq 1; \quad t_n = \frac{r_{n-1}^- - r_{n-1}^+}{\dfrac{1}{r_{n-2}^+} - \dfrac{1}{r_{n-2}^-}}, \quad n \geq 2. \tag{2.4.38}$$

The rest of the argument remains unchanged and gives rise to the following algorithm.

Algorithm 2.11 (Modification by the special quadratic divisor in (2.4.36))
Initialization:

$$\begin{aligned}
&\hat\alpha_0 = x\,\frac{\rho_0^+ + \rho_0^-}{\rho_0^+ - \rho_0^-}\,, \quad \hat\beta_0 = -\frac{1}{2x}\,(\rho_0^+ - \rho_0^-),\\
&\hat\alpha_1 = \alpha_1 - s_2 + s_1, \quad \hat\beta_1 = \beta_1 + s_1(\alpha_0 - \hat\alpha_1) - t_2,\\
&\hat\alpha_2 = \alpha_2 - s_3 + s_2, \quad \hat\beta_2 = \beta_2 + s_2(\alpha_1 - \hat\alpha_2) - t_3 + t_2.
\end{aligned} \tag{2.4.39}$$

Continuation (if $n > 3$): for $k = 3, 4, \ldots, n-1$ do

$$\hat\alpha_k = \alpha_k - s_{k+1} + s_k, \quad \hat\beta_k = \beta_{k-2}\,t_k/t_{k-1}, \tag{2.4.40}$$

where the s_n and t_n are as defined in (2.4.38).

Algorithm 2.11 is implemented in the `OPQ` routine `chri8.m` with two options analogous to those in `chri4.m` and `chri5.m`. Note that $\mathrm{d}\hat\lambda$ in (2.4.36) is negative definite.

2.4.6 *Examples*

The first example is to show an application of the modification algorithm for the special quadratic factor $(t-x)^2$ (cf. the last paragraph of §2.4.3). The next example applies Algorithm 2.8 (just the initialization part) to compute the complex exponential integral. The two examples that follow illustrate the superiority in efficiency of Algorithms 2.8 and 2.9 over the modified Chebyshev algorithm as used in Example 2.49. For zeros close to the support of $\mathrm{d}\lambda$, the respective modified measures $\mathrm{d}\hat\lambda$ and corresponding recurrence coefficients have applications to Gaussian quadrature of functions having poles close to the interval of integration. An illustration of this is given in the remaining two examples.

Example 2.56 *Induced orthogonal polynomials.*

Given an orthogonal polynomial $\pi_m(\,\cdot\,;\mathrm{d}\lambda)$ of fixed degree $m \geq 1$, the sequence of *induced orthogonal polynomials* $\hat\pi_{k,m}(\,\cdot\,) = \pi_k(\,\cdot\,;\pi_m^2\mathrm{d}\lambda)$, $k = 0, 1, 2, \ldots$, has been introduced by Gautschi and Li (1993). Their measure

$$\mathrm{d}\hat\lambda_m(t) = \prod_{\mu=1}^{m}(t - x_\mu)^2\,\mathrm{d}\lambda(t), \tag{2.4.41}$$

where x_μ are the zeros of π_m, modifies the given measure $\mathrm{d}\lambda$ by a product of quadratic factors of the type (2.4.20), so that the routine `chri7.m` can be applied m times in succession to compute the n coefficients $\hat\alpha_{k,m} = \alpha_k(\mathrm{d}\hat\lambda_m)$, $\hat\beta_{k,m} = \beta_k(\mathrm{d}\hat\lambda_m)$, $k = 0, 1, \ldots, n-1$, from the $n+m$ coefficients $\alpha_k = \alpha_k(\mathrm{d}\lambda)$, $\beta_k = \beta_k(\mathrm{d}\lambda)$, $k = 0, 1, \ldots, n-1+m$. This is implemented in the `OPQ` routine `indop.m`. Selected results for the Legendre measure $\mathrm{d}\lambda = \mathrm{d}t$ on $[-1, 1]$, for which

Table 2.22 *Induced Legendre polynomials.*

k	$\hat{\beta}_{k,0}$	$\hat{\beta}_{k,2}$	$\hat{\beta}_{k,6}$	$\hat{\beta}_{k,11}$
0	2.0000000000	0.1777777778	0.0007380787	0.0000007329
1	0.3333333333	0.5238095238	0.5030303030	0.5009523810
6	0.2517482517	0.1650550769	0.2947959861	0.2509913424
12	0.2504347826	0.2467060415	0.2521022519	0.1111727541
19	0.2501732502	0.2214990335	0.2274818789	0.2509466619

$\hat{\alpha}_{k,m} = 0$, are shown in Table 2.22; see the routine `Table2_22.m`. The procedure was found to be remarkably stable, not only for the Legendre measure, but also for other classical measures, and for n and m as large as 320 (see Gautschi (1994, Tables X and XI)).

Example 2.57 *Complex exponential integral*

Let $z \in \mathbb{C}$ be in the complex plane cut along the negative real axis. The exponential integral $E_1(z)$ can be expressed in the form (Abramowitz and Stegun, 1992, eqn 5.1.28)

$$\mathrm{e}^z E_1(z) = \int_0^\infty \frac{\mathrm{e}^{-t}}{t+z}\,\mathrm{d}t,$$

which is simply the Cauchy integral $-\rho_0(-z; \mathrm{e}^{-t}\,\mathrm{d}t)$ for the Laguerre measure. It thus suffices to compute $-r_{-1}(z)$ by the first half of the continued fraction algorithm (2.3.14). The results for $z = r\mathrm{e}^{\mathrm{i}\varphi}$, $r = \frac{1}{2}, 1, 2, 5$ and $\varphi = 0, \pi/4, \pi/2, 3\pi/4$ are shown in Table 2.23 along with the index ν that yields convergence for the

Table 2.23 *Complex exponential integral.*

r	φ	real$(E_1(r\mathrm{e}^{\mathrm{i}\varphi}))$	imag$(E_1(r\mathrm{e}^{\mathrm{i}\varphi}))$	ν
0.5	0.0000	0.559773594774	0.000000000000	104
	0.7854	0.465188800576	–0.489467676815	119
	1.5708	0.177784078811	–1.077688908750	193
	2.3562	–0.232023710149	–1.935271237334	606
1.0	0.0000	0.219383934395	0.000000000000	58
	0.7854	0.099862719160	–0.289974554119	66
	1.5708	–0.337403922900	–0.624713256429	105
	2.3562	–1.233466915671	–1.361233788765	320
2.0	0.0000	0.048900510708	0.000000000000	33
	0.7854	–0.039584645207	–0.082292060497	37
	1.5708	–0.422980828775	0.034616650007	57
	2.3562	–2.169393589174	0.317338393619	166
5.0	0.0000	0.001148295591	0.000000000000	17
	0.7854	–0.002413269237	0.004504243431	19
	1.5708	0.190029749657	–0.020865081850	26
	2.3562	6.311949478582	4.228204825282	66

given error tolerance $\frac{1}{2} \times 10^{-12}$. (To get an accurate reading on the index ν, the routine `cauchy.m` has been altered by letting ν increase in steps of 1 rather than 5.) It can be seen that, as expected, the algorithm has to work harder as z approaches the cut, but less if $|z|$ is large. See the `OPQ` routine `Table2_23.m` used to produce Table 2.23.

Example 2.58 *Modified Chebyshev algorithm vs modification algorithm in the case of linear divisors.*

The routines `gchri1.m` and `chri4.m` were run with $n = 40$ and `eps0`=100× `eps` for Jacobi measures $\mathrm{d}\lambda^{(\alpha,\beta)}$ with parameters $\alpha, \beta = -0.8(0.4)0.8$, $\beta \geq \alpha$; see the `OPQ` routine `Table2_24.m`. Since the results do not differ greatly for different values of the parameters α and β, we show in Table 2.24 only the results for $\alpha = \beta = 0$. In addition to the zero x of the divisor $t - x$, Table 2.24 shows

Table 2.24 *The performance of* `gchri1.m` *and* `chri4.m` *in the case of the Legendre measure.*

x	ν_0	ν	ν_0	ν	discr $\hat{\alpha}$	discr $\hat{\beta}$
–1.001	431	436	392	397	5.00(–16)	8.88(–16)
–1.010	191	196	152	157	2.22(–16)	4.44(–16)
–1.040	135	140	96	101	1.67(–16)	4.44(–16)
–1.070	122	127	83	88	1.67(–16)	4.44(–16)
–1.100	115	120	76	81	1.11(–16)	4.44(–16)

the estimated values ν_0 (provided by the routine `nu0jac.m`) in `gchri1.m` and `chri4.m` and the respective observed values of ν that yield convergence of the continued fraction algorithm (2.3.14) used in the two routines. This is followed by the maximum absolute resp. relative discrepancy between the coefficients $\hat{\alpha}_k$ and $\hat{\beta}_k$ produced by the two routines, the maximum being taken over all k with $0 \leq k \leq 39$. Both routines `gchri1.m` and `chri4.m` produce essentially identical results, but the latter is about five times faster.

Similar phenomena occur in division by a quadratic divisor. This is illustrated in the next example, which uses the routines `gchri2.m` and `chri5.m`.

Example 2.59 *Modified Chebyshev algorithm vs modification algorithm in the case of quadratic divisors.*

Here, we use division by $(t-x)^2+y^2$, where $z = x+\mathrm{i}y$ is taken along the upper half of the ellipse $\mathcal{E}_\rho$ for selected values of ρ. (For the definition of $\mathcal{E}_\rho$, see (2.3.27).) These ellipses are contours of constant ν_0 for Jacobi measures. Information is generated similar to the one in Example 2.58, except that all quantities are averaged over 19 points on $\mathcal{E}_\rho$ corresponding to $\vartheta = j\pi/20$, $j = 1, 2, \ldots, 19$. The results for the Legendre measure are again typical and are shown in Table 2.25 (bars indicate averaging). Both routines `gchri2.m` and `chri5.m` again produce essentially identical results, but the latter is now about five-and-a-half times as fast as the former. See the `OPQ` routine `Table2_25.m`.

Table 2.25 *The performance of* `gchri2.m` *and* `chri5.m` *in the case of the Legendre measure.*

ρ	$\overline{\nu}_0$	$\overline{\nu}$	$\overline{\nu}_0$	$\overline{\nu}$	$\overline{\text{discr}}\,\hat{\alpha}$	$\overline{\text{discr}}\,\hat{\beta}$
1.0500	402	411	363	372	6.18(–15)	1.32(–14)
1.1625	184	192	145	153	1.70(–15)	3.46(–15)
1.2750	144	152	105	113	6.25(–16)	1.37(–15)
1.3875	127	135	88	96	4.40(–16)	9.70(–16)
1.5000	118	125	79	86	2.31(–16)	7.64(–16)

Example 2.60 *Gauss quadrature* of the integral

$$F(x,y) = \int_{-\infty}^{\infty} \mathrm{e}^{-xt} \cos t \, \frac{\mathrm{e}^{-t^2}}{t^2+y^2} \, \mathrm{d}t, \quad y > 0. \tag{2.4.42}$$

Here, $\mathrm{d}\lambda$ is the Hermite measure $\mathrm{d}\lambda(t) = \mathrm{e}^{-t^2}\mathrm{d}t$ on $\mathbb{R}$, and the objective is to compute the recurrence coefficients $\hat{\beta}_k = \beta_k(\mathrm{d}\hat{\lambda})$, where $\mathrm{d}\hat{\lambda}(t) = \mathrm{d}\lambda(t)/(t^2+y^2)$. (By symmetry, $\hat{\alpha}_k = \alpha_k(\mathrm{d}\hat{\lambda}) = 0$ for all k.) Once these coefficients are at hand, we can generate Gauss quadrature rules for $\mathrm{d}\hat{\lambda}$ by the method of §3.1.1 and apply them to the function $f(t) = \mathrm{e}^{-xt}\cos t$. To generate the $\hat{\beta}_k$, we use the routine `chri6.m` with `iopt`=2 (if y is small) and

$$\rho_0'' = -y \int_{-\infty}^{\infty} \frac{\mathrm{e}^{-t^2}}{t^2+y^2} \, \mathrm{d}t = -\pi \mathrm{e}^{y^2} \operatorname{erfc} y$$

(cf. Abramowitz and Stegun (1992, eqn 7.4.11)). Since $F(x,y)$ is an even function in both x and y, it suffices to consider positive values of x and y. Results, produced by the `OPQ` routine `Table2_26.m`, are shown in Table 2.26 for $y = 0.1, 0.01$, and 0.001, and selected values of x. The upper number in each entry represents the relative error of the n-point Gauss formula relative to $\mathrm{d}\hat{\lambda}$ applied to $f(t) = \mathrm{e}^{-xt}\cos t$, while the lower number is the relative error of the n-point Gauss–Hermite formula applied to $f(t) = \mathrm{e}^{-xt}\cos t/(t^2+y^2)$. The last column shows "exact" values, which, in the absence of explicit (or even approximate analytic) results, were taken to be the values to which our Gauss formula for $\mathrm{d}\hat{\lambda}$ were observed to converge in quadruple-precision arithmetic. We used Maple to compute ρ_0'' to the same precision. (The procedure in `chri6.m` with `iopt`=1 does not converge for such small values of y.)

The superiority of the specially constructed Gauss formula over the classical Gauss–Hermite formula is impressive, although the latter does fairly well when $|x|$ is large.

Example 2.61 The integral

$$G(x,y,a) = \int_{-\infty}^{\infty} J_0(at) \frac{\mathrm{e}^{-t^2}}{(t-x)^2+y^2} \, \mathrm{d}t,$$

where J_0 is the Bessel function of order zero.

Table 2.26 *Gauss quadrature for the integral in (2.4.42).*

y	$x\backslash n$	5	10	20	40	80	"exact"
.1	1.0	1.3(–07)	1.7(–14)				2.80191134379093(1)
		2.4(+00)	6.5(–01)	4.9(–01)	3.2(–01)	1.7(–01)	
	2.0	2.3(–05)	2.1(–10)	9.5(–16)			2.98880485427655(1)
		2.2(+00)	6.0(–01)	4.5(–01)	3.0(–01)	1.5(–01)	
	5.0	2.9(+00)	9.2(–03)	5.6(–09)	2.7(–14)		–2.32413409260872(1)
		4.1(+00)	6.9(–01)	5.2(–01)	3.4(–01)	1.8(–01)	
	10.0	1.0(+00)	1.9(+00)	1.4(+00)	3.1(–08)	2.4(–13)	3.12274649146902(8)
		1.0(+00)	2.7(+00)	8.5(–01)	8.7(–09)	8.1(–09)	
.01	1.0	1.2(–08)	2.4(–15)				3.10499175120235(2)
		2.9(+01)	9.7(–01)	9.5(–01)	9.2(–01)	8.8(–01)	
	2.0	2.3(–06)	2.1(–11)	0.0(+00)			3.12740540639842(2)
		2.9(+01)	9.6(–01)	9.4(–01)	9.1(–01)	8.8(–01)	
	5.0	2.6(–01)	8.2(–04)	5.0(–10)	6.1(–15)		2.62429881105967(2)
		3.5(+01)	1.1(+00)	1.1(+00)	1.1(+00)	1.0(+00)	
	10.0	1.0(+00)	1.9(+00)	1.4(+00)	3.2(–08)	8.8(–15)	3.11965015566419(8)
		1.0(+00)	2.7(+00)	8.5(–01)	9.1(–07)	8.8(–07)	
.001	1.0	1.2(–09)	2.9(–16)				3.13790449274505(3)
		3.0(+02)	1.0(+00)	9.9(–01)	9.9(–01)	9.9(–01)	
	2.0	2.3(–07)	2.1(–12)	4.3(–16)			3.14018771045802(3)
		3.0(+02)	1.0(+00)	9.9(–01)	9.9(–01)	9.9(–01)	
	5.0	2.2(–02)	7.0(–05)	4.3(–11)	2.9(–16)		3.09017266953282(3)
		3.0(+02)	1.0(+00)	1.0(+00)	1.0(+00)	1.0(+00)	
	10.0	1.0(+00)	1.9(+00)	1.4(+00)	3.2(–08)	5.0(–14)	3.11964740917142(8)
		1.0(+00)	2.7(+00)	8.5(–01)	1.0(–05)	9.9(–06)	

When $z = x + \mathrm{i}y$ is not too close to the real axis, we can use the routine `chri5.m` (with `iopt`=1) to first generate the three-term recurrence coefficients of the modified Hermite measure $\mathrm{d}\hat{\lambda}(t) = \mathrm{e}^{-t^2}/((t-x)^2 + y^2)$ from the known Hermite recurrence coefficients, and then generate the respective Gauss quadrature rules to evaluate G. For the purpose of illustration, we take $x = 2$, $y = 1$, $a = 7.5$, and set the error tolerance at `eps0`$=\frac{1}{2} \times 10^{-8}$. The point $z = 2 + \mathrm{i}$ is sufficiently close to the real axis to require a relatively large value of ν in the continued fraction algorithm (2.3.14), for example, $\nu = 186$ if $n = 40$. On the other hand, these special Gauss quadrature approximations to G converge considerably faster than, for example, classical Gauss–Hermite quadrature; see Table 2.27, produced by the `OPQ` routine `Table2_27.m`.

More spectacular improvements can be had if $z = x + \mathrm{i}y$ is very close to the real axis so that forward recursion is an option. We illustrate this for $x = 0$, $y > 0$, and the same value $a = 7.5$, noting from Example 2.60 that $\rho_0' = 0$, $\rho_0'' = -\pi \mathrm{e}^{y^2} \operatorname{erfc} y$ in this case. Results for $y = 0.1$ are shown in Table 2.28 calculated by `chri6.m` with option `iopt`=2; see the `OPQ` routine `Table2_28.m`.

Table 2.27 *n-point Gauss quadrature for* $G(2, 1, 7.5)$.

n	Modified Hermite	Hermite
5	–0.01...	0.2...
10	0.041...	0.01...
15	0.0546...	0.052...
20	0.053863...	0.0536...
25	0.05386989...	0.05382...
30	0.05386988457...	0.05385...
35	0.053869884583	0.053866...
40	0.053869884583	0.0538696...

Table 2.28 *n-point Gauss quadrature for* $G(0, .1, 7.5)$.

n	Modified Hermite	Hermite
5	22.7...	94.7...
10	19.7...	–0.6...
15	19.966...	55.4...
20	19.96350...	4.1...
25	19.96352269...	42.8...
30	19.96352266624...	7.3...
35	19.963522666263	36.5...
40	19.963522666263	9.6...

The alternately large and small results for n odd resp. n even in the last column of Table 2.28 are due to the presence of a zero node in the Gauss–Hermite quadrature rule when n is odd, which causes the second factor in the integrand of G to peak at the value 10^2.

2.5 Computing Sobolev orthogonal polynomials

The literature on Sobolev orthogonal polynomials (cf. Definition 1.58) is quite extensive, but attention has been directed largely to algebraic and analytic properties. Results of a numerical nature are practically nonexistent. An attempt, however, has been made to extend moment-based methods (§2.1) and discretization methods (§2.2) to general orthogonal polynomials of Sobolev type; see Gautschi and Zhang (1995). This requires a rather formidable technical apparatus, especially for moment-based methods, and we will therefore limit ourselves in the following to describing the principal ideas underlying the computational procedures, just enough for the reader to be able to make intelligent use of the Matlab routines that implement these procedures.

We recall from §1.7 that Sobolev inner products involve derivatives and are of the form

$$(u, v)_S = (u, v)_{\mathrm{d}\lambda_0} + (u', v')_{\mathrm{d}\lambda_1} + \cdots + (u^{(s)}, v^{(s)})_{\mathrm{d}\lambda_s}, \quad s \geq 1, \tag{2.5.1}$$

where $\mathrm{d}\lambda_\sigma$ are positive measures. (For notations, see §1.1.1.) Sobolev polynomials $\pi_k(\,\cdot\,) = \pi_k(\,\cdot\,; S)$ are orthogonal with respect to this inner product (cf. Definition 1.58). The objective is to compute the upper Hessenberg matrix of order n,

$$\boldsymbol{H}_n = \begin{bmatrix} \beta_0^0 & \beta_1^1 & \beta_2^2 & \cdots & \beta_{n-2}^{n-2} & \beta_{n-1}^{n-1} \\ 1 & \beta_0^1 & \beta_1^2 & \cdots & \beta_{n-3}^{n-2} & \beta_{n-2}^{n-1} \\ 0 & 1 & \beta_0^2 & \cdots & \beta_{n-4}^{n-2} & \beta_{n-3}^{n-1} \\ \vdots & \vdots & \vdots & & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & \beta_0^{n-2} & \beta_1^{n-1} \\ 0 & 0 & 0 & \cdots & 1 & \beta_0^{n-1} \end{bmatrix}, \tag{2.5.2}$$

the entries β_j^k of which allow us to express, and thus to compute, the (monic) Sobolev orthogonal polynomial of degree $k+1$ in terms of those of lower degree,

$$\pi_{k+1}(t) = t\pi_k(t) - \sum_{j=0}^{k} \beta_j^k \pi_{k-j}(t), \quad k = 0, 1, 2, \ldots, n-1. \tag{2.5.3}$$

In possession of the matrix $\boldsymbol{H}_n$, we will also have access to the zeros $\tau_1, \tau_2, \ldots, \tau_n$ of $\pi_n(\,\cdot\,; S)$, these being the eigenvalues of $\boldsymbol{H}_n$ (see Theorem 1.65).

2.5.1 *Algorithm based on moment information*

Having to deal with $s+1$ different measures $\mathrm{d}\lambda_\sigma$, $\sigma = 0, 1, \ldots, s$, we introduce $s+1$ sets of modified moments in accordance with (2.1.23),

$$m_k^{(\sigma)} = \int_{\mathbb{R}} p_k(t)\, \mathrm{d}\lambda_\sigma(t), \quad k = 0, 1, 2, \ldots, \quad \sigma = 0, 1, \ldots, s. \tag{2.5.4}$$

For simplicity, we use the same sequence of polynomials p_k for each measure $\mathrm{d}\lambda_\sigma$ and assume, as in Example 2.8, that they are orthogonal with respect to some measure $\mathrm{d}\ell$, hence satisfy a three-term recurrence relation

$$\begin{gathered} p_{k+1}(t) = (t - a_k)p_k(t) - b_k p_{k-1}(t), \quad k = 0, 1, 2, \ldots, \\ p_{-1}(t) = 0, \quad p_0(t) = 1. \end{gathered} \tag{2.5.5}$$

An algorithm can then be developed (Gautschi and Zhang, 1995, §2), resembling the modified Chebyshev algorithm of §2.1.7, that *takes as input the first* $2n$ *coefficients* a_k, b_k, $0 \le k \le 2n-1$, *of (2.5.5), the modified moments* $m_k^{(0)}$, $0 \le k \le 2n-1$, *and* $m_k^{(\sigma)}$, $0 \le k \le 2n-2$ *(if* $n \ge 2$*),* $1 \le \sigma \le s$, *of (2.5.4), and computes from them the matrix* $\boldsymbol{H}_n$ *in (2.5.2).* The complexity of the algorithm is $O(n^3)$, which is one order higher than the one for the modified Chebyshev algorithm for ordinary orthogonal polynomials.

As in the modifed Chebyshev algorithm, important ingredients of the algorithm are the "mixed moments" $\sigma_{k\ell} = (\pi_k, p_\ell)_S$, now relative to the Sobolev inner product (2.5.1). These, in turn, require for their computation "mixed derivative moments" $\mu_{k,\ell,\sigma}^{(i,j)} = (\pi_k^{(i)}, p_\ell^{(j)})_{\mathrm{d}\lambda_\sigma}$, $\sigma = 1, 2, \ldots, s$, $i, j \le \sigma$, relative to the

individual inner products involving derivatives in (2.5.1). Accordingly, there will be a tableau containing the mixed moments $\sigma_{k\ell}$ much like the tableau in Fig. 2.1, and for each i, j, and σ, another auxiliary tableau containing the mixed derivative moments. Both have the trapezoidal shape of Fig. 2.1, but the latter with height $n-2$ instead of $n-1$. Each quantity in these tableaux is computed recursively in terms of the three nearest quantities on the next lower level, and in terms of all quantities vertically below. The initialization of these tableaux engages the modified moments (2.5.4), since $\sigma_{0\ell} = m_\ell^{(0)}$ and $\mu_{0,\ell,\sigma}^{(0,0)} = m_\ell^{(\sigma)}$, $\sigma \geq 1$, but the complete initialization of all the quantities $\mu_{0,\ell,\sigma}^{(i,j)}$ is a rather involved process. Once the tableau for the $\sigma_{k\ell}$ has been computed, one obtains first

$$\beta_0^0 = \frac{\sigma_{01}}{\sigma_{00}} + a_0, \tag{2.5.6}$$

and then, successively, for $k = 1, 2, \ldots, n-1$,

$$\begin{aligned}
\beta_0^k &= \frac{\sigma_{k,k+1}}{\sigma_{kk}} + a_k - \frac{\sigma_{k-1,k}}{\sigma_{k-1,k-1}}\,, \\
\beta_{k-j}^k &= \frac{\sigma_{j,k+1}}{\sigma_{jj}} + a_k \frac{\sigma_{jk}}{\sigma_{jj}} + b_k \frac{\sigma_{j,k-1}}{\sigma_{jj}} - \frac{\sigma_{j-1,k}}{\sigma_{j-1,j-1}} - \sum_{\ell=j}^{k-1} \beta_{\ell-j}^\ell \frac{\sigma_{\ell k}}{\sigma_{\ell\ell}}\,, \\
&\qquad\qquad j = k-1, k-2, \ldots, 1 \quad (\text{if } k \geq 2), \\
\beta_k^k &= \frac{\sigma_{0,k+1}}{\sigma_{00}} + a_k \frac{\sigma_{0k}}{\sigma_{00}} + b_k \frac{\sigma_{0,k-1}}{\sigma_{00}} - \sum_{\ell=0}^{k-1} \beta_\ell^\ell \frac{\sigma_{\ell k}}{\sigma_{\ell\ell}}\,,
\end{aligned} \tag{2.5.7}$$

where a_k and b_k are the coefficients in (2.5.5).

The procedure is implemented for $s = 1$ in the `OPQ` routine `chebyshev_sob.m`. It takes as input arguments, apart from the parameter n, the $2 \times (2n)$ array `mom` containing the first $2n$ modified moments $m_k^{(\sigma)}$, $k = 0, 1, \ldots, 2n-1$, $\sigma = 0, 1$, of the two measures $\mathrm{d}\lambda_0$ and $\mathrm{d}\lambda_1$, and the $(2n-1) \times 2$ array `abm` of the first $2n-1$ coefficients a_k, b_k, $k = 0, 1, \ldots, 2n-2$ in (2.5.5). A call to the routine thus has the form

$$[\mathtt{B}, \mathtt{normsq}] = \mathtt{chebyshev\_sob}(\mathtt{n}, \mathtt{mom}, \mathtt{abm})$$

where the output argument `B` is the $n \times n$ upper triangular matrix of the coefficients β_j^k, $0 \leq j \leq k$, $0 \leq k \leq n-1$, with β_j^k occupying the position $(j+1, k+1)$ in the matrix, and `normsq` is the n-vector of the squared norms $\|\pi_k(\,\cdot\,; S)\|^2$, $k = 0, 1, \ldots, n-1$. If the input argument `abm` is omitted, the routine assumes `abm=zeros(2*n-1,2)`, that is, ordinary moments.

A large class of Sobolev orthogonal polynomials, in particular those originally introduced in the early 1960s, correponds to the case $s = 1$ and depends essentially on one measure only, by virtue of

$$\mathrm{d}\lambda_0(t) = \mathrm{d}\lambda(t), \quad \mathrm{d}\lambda_1(t) = \gamma\, \mathrm{d}\lambda(t), \quad \gamma > 0. \tag{2.5.8}$$

In the limit as $\gamma \downarrow 0$, one recovers the ordinary orthogonal polynomials.

Example 2.62 The *polynomials of Althammer*.

These are the Sobolev orthogonal polynomials in the "Legendre case" of (2.5.8), that is, $\mathrm{d}\lambda(t) = \mathrm{d}t$ on $[-1,1]$, first studied by Althammer (1962). To indicate their dependence on the parameter γ, we denote them here by $\pi_n(\,\cdot\,) = \pi_n(\,\cdot\,;\gamma)$. As $\gamma \downarrow 0$, they approach the Legendre polynomials, and as $\gamma \to \infty$, up to the factor t^2-1, the (monic) Jacobi polynomials with parameters $\alpha = \beta = 1$ (cf. Cohen (1975)),

$$\pi_n(t;\gamma) \to (t^2-1)\pi_{n-2}^{(1,1)}(t) \quad \text{as } \gamma \to \infty, \quad n \geq 2. \tag{2.5.9}$$

We illustrate this by computing the matrix `B` of order $n = 21$ for the Althammer polynomials with parameter $\gamma = 100$. We choose the (monic) Legendre polynomials in the role of the p_k in (2.5.5), so that all modified moments are zero except for $m_0^{(0)} = 2$ and $m_0^{(1)} = 2\gamma$. The following Matlab script accomplishes the task:

```
n=21; g=100;
mom=zeros(2,2*n); mom(1,1)=2; mom(2,1)=2*g;
abm=r_jacobi(2*n-1);
B=chebyshev_sob(n,mom,abm);
```

Since the polynomials π_k on the right of (2.5.9) satisfy the recurrence relation $\pi_{k+1}(t) = t\pi_k(t) - \beta_{k-2}^{(1,1)}\pi_{k-1}(t)$, where $\beta_0^{(1,1)}, \beta_1^{(1,1)}, \ldots$ are the recurrence coefficients of the Jacobi polynomials in question, one expects, for large γ, that $\beta_1^k \approx \beta_{k-2}^{(1,1)}$ and $\beta_j^k \approx 0$ for $j \geq 2$. This is confirmed in Table 2.29; see the `OPQ` routine `Table2_29.m`.

Table 2.29 *The behavior of β_j^k for large γ (=100).*

k	β_1^k	$\max_{2\leq j\leq k}\lvert\beta_j^k\rvert$	$\beta_{k-2}^{(1,1)}$
5	.23813...	3.62(–5)	.23809...
10	.247680...	8.96(–7)	.247678...
15	.24904270...	1.80(–7)	.24904214...
20	.24948046...	6.34(–8)	.24948024...

2.5.2 *Stieltjes-type algorithm*

The idea, here, is to extend the Stieltjes procedure of §2.2.3.1 to Sobolev orthogonal polynomials, combining formula (1.7.5) of Theorem 1.63,

$$\beta_j^k = \frac{(t\pi_k, \pi_{k-j})_S}{(\pi_{k-j}, \pi_{k-j})_S}, \quad j = 0, 1, \ldots, k; \quad k = 0, 1, \ldots, n-1, \tag{2.5.10}$$

with the recurrence relation (2.5.3). Specifically, the inner products in both numerator and denominator of (2.5.10) are evaluated by numerical quadrature. Since they involve polynomials of degree at most $2n-1$, they can be computed exactly by appropriate n-point Gauss quadrature rules. The polynomials

themselves, and their derivatives, are computed recursively by (2.5.3) and its differentiated version, employing coefficients β_j^k already computed. Thus, initially, by (2.5.10) and the definition (2.5.1) of the Sobolev inner product,

$$\beta_0^0 = \frac{(t,1)_S}{(1,1)_S} = \frac{(t,1)_{\mathrm{d}\lambda_0}}{(1,1)_{\mathrm{d}\lambda_0}} = \alpha_0(\mathrm{d}\lambda_0).$$

Assuming $\alpha_0(\mathrm{d}\lambda_0)$ to be known, we can use β_0^0 to compute π_1 from (2.5.3). With π_0 and π_1 both at hand, formula (2.5.10) allows us to compute β_0^1 and β_1^1, which, in turn, can be used in (2.5.3) to compute π_2. In this way, much like in the Stieltjes procedure for ordinary orthogonal polynomials, we can continue, using alternately (2.5.10) and (2.5.3), to successively generate π_k, and thus β_j^k, $0 \le j \le k$, up to $k = n-1$.

The procedure is much simpler, conceptually, than the moment-based algorithm of §2.5.1, but is considerably slower, being, in general, of complexity $O(n^4)$. The procedure has been observed, however, to often provide better accuracy.

In the `OPQ` routine `stieltjes_sob.m` that implements this procedure for any $s \ge 1$, it is assumed that each measure $\mathrm{d}\lambda_\sigma$ consists of an absolutely continuous part, $\mathrm{d}\lambda_\sigma^{\mathrm{ac}}$, and a discrete part, $\mathrm{d}\lambda_\sigma^{\mathrm{dis}}$,

$$\mathrm{d}\lambda_\sigma(t) = \mathrm{d}\lambda_\sigma^{\mathrm{ac}}(t) + \mathrm{d}\lambda_\sigma^{\mathrm{dis}}(t), \quad \sigma = 0, 1, \ldots, s, \tag{2.5.11}$$

where one or the other could possibly be empty, and

$$\mathrm{d}\lambda_\sigma^{\mathrm{dis}}(t) = \sum_{\rho=1}^{r_\sigma} y_\rho^{(\sigma)} \delta(t - t_\rho^{(\sigma)})\,\mathrm{d}t, \quad y_\rho^{(\sigma)} > 0, \tag{2.5.12}$$

with $\delta(\,\cdot\,)$ the delta function. The basic assumption in the design of the routine `stieltjes_sob.m` is that for each measure $\mathrm{d}\lambda_\sigma$, an n_σ-point quadrature rule

$$\int_{\mathbb{R}} p(t)\,\mathrm{d}\lambda_\sigma(t) = \sum_{\nu=1}^{n_\sigma} \lambda_\nu^{(\sigma)} p(\tau_\nu^{(\sigma)}), \quad p \in \mathbb{P}_{2(n-\sigma)-1}, \quad \sigma = 0, 1, \ldots, s, \tag{2.5.13}$$

be available that integrates polynomials exactly up to degree $2(n-\sigma)-1$. These quadrature rules, in fact, constitute the principal information, apart from the parameters n, s, and $\alpha_0(\mathrm{d}\lambda_0)$, which must be furnished as input to the routine. This is done by means of two arrays, `nd` and `xw`. The first is a vector of dimension $s+1$, having the number of points in the quadrature rules (2.5.13) as components,

$$\mathtt{nd} = [n_0, n_1, \ldots, n_s].$$

The other array, `xw`, is an array of dimension $N \times (2s+2)$, where $N = \max_{0 \le \sigma \le s} n_\sigma$, and contains the nodes and weights of the quadrature rules,

$$\mathtt{xw} = \begin{bmatrix} \tau_1^{(0)} & \tau_1^{(1)} & \cdots & \tau_1^{(s)} & \lambda_1^{(0)} & \lambda_1^{(1)} & \cdots & \lambda_1^{(s)} \\ \tau_2^{(0)} & \tau_2^{(1)} & \cdots & \tau_2^{(s)} & \lambda_2^{(0)} & \lambda_2^{(1)} & \cdots & \lambda_2^{(s)} \\ \tau_3^{(0)} & \tau_3^{(1)} & \cdots & \tau_3^{(s)} & \lambda_3^{(0)} & \lambda_3^{(1)} & \cdots & \lambda_3^{(s)} \\ \vdots & \vdots & & \vdots & \vdots & \vdots & & \vdots \end{bmatrix} \in \mathbb{R}^{N\times(2s+2)}.$$

In each column of `xw` the entries after $\tau_{n_\sigma}^{(\sigma)}$ resp. $\lambda_{n_\sigma}^{(\sigma)}$ (if any) are not used by the routine. There is finally a logical input variable, `same`, which has to be set equal to 1 if $n_0 = n_1 = \cdots = n_s = N$ and $\tau_\nu^{(0)} = \tau_\nu^{(1)} = \cdots = \tau_\nu^{(s)}$ for $\nu = 1, 2, \ldots, N$, that is, if all quadrature rules have the same nodes. Otherwise, `same` has to be set equal to 0. The role of this parameter is to switch to a simplified, and thus faster, procedure if `same`=1. A call to the routine, therefore, has the form

$$[\mathtt{B}, \mathtt{normsq}] = \mathtt{stieltjes\_sob}(\mathtt{n}, \mathtt{s}, \mathtt{nd}, \mathtt{xw}, \mathtt{a0}, \mathtt{same})$$

with `B` and `normsq` having the same meaning as in the routine `chebyshev_sob.m` of §2.5.1.

Here are three typical setups for handling measures like (2.5.11):

(1) Use an $(n-\sigma)$-point Gauss rule relative to the measure $\mathrm{d}\lambda_\sigma^{\mathrm{ac}}$ to integrate $\int_{\mathbb{R}} p(t)\,\mathrm{d}\lambda_\sigma^{\mathrm{ac}}(t)$ and then add on the contribution $\int_{\mathbb{R}} p(t)\,\mathrm{d}\lambda_\sigma^{\mathrm{dis}}(t)$ from the discrete part of the measure. This will produce a quadrature rule (2.5.13) with $n_\sigma = n - \sigma + r_\sigma$, where the first $n-\sigma$ terms come from the Gauss rule for $\mathrm{d}\lambda_\sigma^{\mathrm{ac}}$ and the remaining terms from the discrete measure $\mathrm{d}\lambda_\sigma^{\mathrm{dis}}$.

(2) Use an $(n-\sigma)$-point Gauss rule for the entire measure $\mathrm{d}\lambda_\sigma$. In this case, $n_\sigma = n - \sigma$.

(3) If all measures $\mathrm{d}\lambda_\sigma$ are the same except for constant positive factors, use the same n-point Gauss rule for all of them, multiplied by the appropriate factors, either for the absolutely continuous part of the measure or for the entire measure. In this case, $n_\sigma = n + r$ resp. $n_\sigma = n$, where r is the common value of the r_σ.

The third setup, for example, is one that is appropriate for the Althammer polynomials of Example 2.62. This gives rise to the script `althammer.m`:

```
n=21; g=100; s=1; nd=[n n]; a0=0; same=1;
ab=r_jacobi(n); zw=gauss(n,ab);
xw=[zw(:,1) zw(:,1) zw(:,2) g*zw(:,2)];
B=stieltjes_sob(n,s,nd,xw,a0,same);
```

The results produced are the same as those in Table 2.29.

2.5.3 *Zeros*

All the nice properties known for the zeros of ordinary orthogonal polynomials (cf. §1.2.2) do not necessarily carry over to Sobolev orthogonal polynomials. This is why much of the recent and current literature on Sobolev orthogonal polynomials is devoted to a study of their zeros. In this regard, computational methods are an important exploratory tool (see, e.g. Gautschi and Zhang (1995,

§3.2–3.4)). According to Theorem 1.65, the zeros $\tau_1, \tau_2, \ldots, \tau_n$ of $\pi_n(\,\cdot\,; S)$ can be computed as the eigenvalues of the matrix $\boldsymbol{H}_n$ of (2.5.2). This is implemented in the `OPQ` routine `sobzeros.m`, having the calling sequence

$$\mathtt{z} = \mathtt{sobzeros}(\mathtt{n}, \mathtt{N}, \mathtt{B})$$

where `B` is the matrix returned by `chebyshev_sob.m` or `stieltjes_sob.m`, and `z` is the n-vector of the zeros of the Sobolev orthogonal polynomial of degree n, $1 \le n \le N$. For large n, the eigenvalues of $\boldsymbol{H}_n$ are potentially ill-conditioned.

We illustrate the routine in two examples. The first, due to Meijer (1994), is an example of Sobolev orthogonal polynomials that have only a few real zeros.

Example 2.63 The Sobolev inner product

$$(u, v)_S = \int_{-1}^{3} u(t)v(t)\,\mathrm{d}t + \gamma \int_{-1}^{1} u'(t)v'(t)\,\mathrm{d}t + \int_{1}^{3} u'(t)v'(t)\,\mathrm{d}t, \quad \gamma > 0. \tag{2.5.14}$$

Meijer (1994) proved that for $n\,(\text{even}) \ge 2$ and γ *sufficiently large*, the Sobolev orthogonal polynomial $\pi_n(\,\cdot\,; S)$ has exactly two real zeros, one in $[-3, -1]$, the other in $[1, 3]$. Likewise, if $n\,(\text{odd}) \ge 3$, there is exactly one real zero, located in $[1, 3]$, if γ is sufficiently large. We can use our numerical methods to explore what, concretely, "sufficiently large" means, and what happens when γ is not sufficiently large. We will do this for $2 \le n \le 6$ with the help of the routines `stieltjes_sob.m` and `sobzeros.m`. We have $s = 1$ and $\mathrm{d}\lambda_0(t) = \mathrm{d}t$ on $[-1, 3]$, $\mathrm{d}\lambda_1(t) = \gamma\,\mathrm{d}t$ if $t \in [-1, 1]$, and $\mathrm{d}\lambda_1(t) = \mathrm{d}t$ if $t \in (1, 3]$. We then write

$$\int p(t)\,\mathrm{d}\lambda_0(t) = 2\int_{-1}^{1} p(2x+1)\,\mathrm{d}x, \quad \int p(t)\,\mathrm{d}\lambda_1(t) = \int_{-1}^{1} [\gamma p(x) + p(x+2)]\,\mathrm{d}x$$

and apply n-point Gauss–Legendre quadrature to the integrals on the right-hand sides. This requires $\mathtt{nd} = [n, 2n]$ and calls for an array `xw` of the form

$$\mathtt{xw} = \begin{bmatrix} 2\tau_1^G + 1 & \tau_1^G & 2\lambda_1^G & \gamma\lambda_1^G \\ \vdots & \vdots & \vdots & \vdots \\ 2\tau_n^G + 1 & \tau_n^G & 2\lambda_n^G & \gamma\lambda_n^G \\ & \tau_1^G + 2 & & \lambda_1^G \\ & \vdots & & \vdots \\ & \tau_n^G + 2 & & \lambda_n^G \end{bmatrix} \in \mathbb{R}^{2n\times 4},$$

where τ_ν^G, λ_ν^G are the nodes and weights of the Gauss–Legendre quadrature rule. Furthermore, $\alpha_0(\mathrm{d}\lambda_0) = 1$, and $\mathtt{same} = 0$. We are now ready to call the routine `stieltjes_sob.m` to generate the matrix `B` and `sobzeros.m` to compute the zeros of $\pi_n(\,\cdot\,; S)$. This is done in the `OPQ` routine `Example2_63.m`, the core of which looks as follows:

```
N=6; s=1; a0=1; same=0; nd=[N 2*N];
for g=[43646.1 43646.2]
   ab=r_jacobi(N); zw=gauss(N,ab);
   xw=zeros(2*N,2*(s+1));
   xw(1:N,1)=2*zw(:,1)+1; xw(1:N,2)=zw(:,1);
   xw(1:N,3)=2*zw(:,2); xw(1:N,4)=g*zw(:,2);
   xw(N+1:2*N,2)=zw(:,1)+2; xw(N+1:2*N,4)=zw(:,2);
   B=stieltjes_sob(N,s,nd,xw,a0,same);
   z=sobzeros(N,N,B)
end
```

Experimenting with this routine for various values of n and γ, we were able to obtain the more concrete information, displayed in Table 2.30, about the zeros of the respective Sobolev polynomials. It can be seen that the distribution of zeros

Table 2.30 *Zeros of the Sobolev polynomials orthogonal with respect to the inner product in (2.5.14).*

n	γ	Real zeros
2	$0 \le \gamma \le 10.333$	2 real zeros
	$10.334 \le \gamma < \infty$	2 real zeros in $[-3,-1] \cup [1,3]$
4	$0 \le \gamma \le 7.4773$	4 real zeros
	$7.4774 \le \gamma \le 61.745$	2 real zeros
	$61.746 \le \gamma \le 153.23$	4 real zeros
	$153.24 \le \gamma < \infty$	2 real zeros in $[-3,-1] \cup [1,3]$
6	$0 \le \gamma \le 45.011$	6 real zeros
	$45.012 \le \gamma \le 50.226$	4 real zeros
	$50.227 \le \gamma \le 41868.5$	2 real zeros
	$41868.6 \le \gamma \le 42155.5$	4 real zeros
	$42155.6 \le \gamma \le 43512.6$	6 real zeros
	$43512.7 \le \gamma \le 43646.1$	4 real zeros
	$43646.2 \le \gamma < \infty$	2 real zeros in $[-3,-1] \cup [1,3]$
3	$0 \le \gamma \le 21.461$	3 real zeros
	$21.462 \le \gamma < \infty$	1 real zero in $[1,3]$
5	$0 \le \gamma \le 10.193$	5 real zeros
	$10.194 \le \gamma \le 1811.7$	3 real zeros
	$1811.8 \le \gamma \le 2153.6$	5 real zeros
	$2153.7 \le \gamma \le 2183.4$	3 real zeros
	$2183.5 \le \gamma < \infty$	1 real zero in $[1,3]$

is rather complicated for values of γ before the theorem of Meijer takes hold.

In the next example, we will have occasion to combine the present routines with earlier ones to explore the existence and location of complex zeros for certain Sobolev orthogonal polynomials of Gegenbauer type.

Example 2.64 The Sobolev inner product

$$(u,v)_S = \int_{-1}^{1} u(t)v(t)(1-t^2)^{\alpha-1}\,\mathrm{d}t + \gamma \int_{-1}^{1} u'(t)v'(t)\,\frac{(1-t^2)^{\alpha}}{t^2+y^2}\,\mathrm{d}t, \quad \alpha > 0. \tag{2.5.15}$$

Groenevelt (2002, Theorem 5.9) proved that in the case $\gamma \to \infty$ the Sobolev orthogonal polynomials of even degree $n \geq 4$ have complex zeros if $y < y_0$ and y_0 is *sufficiently small*. Could it be that this is also true for finite values of γ? We explore, and seem to confirm, this in the case $\gamma = 1$ and $\alpha = \frac{1}{2}$ and at the same time try to determine what "sufficiently small" means for $n = 4, 6, \ldots, 12$. To apply our routine `sobzeros.m`, we must first determine the matrix `B` that goes with the inner product (2.5.15). We compute it with `stieltjes_sob.m`, noting that $\mathrm{d}\lambda_0(t) = (1-t^2)^{\alpha-1}\,\mathrm{d}t$ is a Gegenbauer measure for which the Gauss quadrature rules are easily generated, while $\mathrm{d}\lambda_1(t) = (1-t^2)^{\alpha}\,\mathrm{d}t/(t^2+y^2)$ calls for Algorithm 2.10 to obtain its recurrence coefficients and hence the required Gauss quadrature rules. Either option in Algorithm 2.10 can be used, the one with `iopt=1` being more computer intensive, but returns more accurate answers. This is all put together in the routine `Example2_64.m`, the core of which has the following appearance:

```
N=12; s=1; same=0; eps0=1000*eps; numax=1000; nd=[N N]:
alpha=.5;
for y=[.0914 .0913 .09 .07 .03]
   ab0=r_jacobi(numax,alpha);
   z=complex(0,y);
   nu0=nu0jac(0,z,eps0);
   iopt=1; rho0=0;
   ab1=chri6(N,ab0,y,eps0,nu0,numax,rho0,iopt);
   zw1=gauss(N,ab1);
   ab=r_jacobi(N,alpha-1); zw=gauss(N,ab);
   xw=[zw(:,1) zw1(:,1) zw(:,2) zw1(:,2)];
   a0=ab(1,1);
   B=stieltjes_sob(N,s,nd,xw,a0,same);
   z=sobzeros(N,N,B)
end
```

The routine is used to determine lower and upper bounds of y_0 for $n = 4, 6, \ldots, 12$. These are shown in Table 2.31.

Similar results are observed for other values of α, for example, $\alpha = \frac{1}{4}, \frac{3}{4}, 1, \frac{3}{2}$, and 2. When complex zeros occur, they are purely imaginary.

2.5.4 *Finite expansions in Sobolev orthogonal polynomials*

In some applications, for example, least squares approximation (cf. §3.2.3), one needs to evaluate finite sums in Sobolev orthogonal polynomials,

Table 2.31 *Complex zeros of the Sobolev polynomials orthogonal with respect to the inner product in (2.5.15).*

n	Lower bound of y_0	Upper bound of y_0
4	0.2975	0.2976
6	0.2065	0.2066
8	0.1449	0.1450
10	0.1119	0.1120
12	0.0913	0.0914

$$r(t) = \sum_{j=0}^{n} c_j \pi_j(t), \tag{2.5.16}$$

and, perhaps, some of their derivatives as well. Here, π_j satisfy the recurrence relation (2.5.3), with coefficients β_j^k taken from the columns of the matrix $\boldsymbol{H}_n$ of (2.5.2). An algorithm for doing this efficiently, which resembles Clenshaw's algorithm for ordinary orthogonal polynomials, can be developed as follows.

Suppose we want to evaluate $r(t)$ and its first s derivatives. We write the recurrence relation (2.5.3) for the Sobolev orthogonal polynomials, and the recurrence relations obtained from it by repeated differentiation, in matrix form as

$$\boldsymbol{L}\boldsymbol{\pi}(t) = \boldsymbol{\rho}, \tag{2.5.17}$$

where $\boldsymbol{\pi} = \boldsymbol{\pi}(t)$ and $\boldsymbol{\rho} = \boldsymbol{\rho}(t)$ are the $(n+1) \times (s+1)$ matrices

$$\boldsymbol{\pi} = \begin{bmatrix} \pi_0 & 0 & 0 & \cdots & 0 \\ \pi_1 & \pi_1' & 0 & \cdots & 0 \\ \pi_2 & \pi_2' & \pi_2'' & \cdots & 0 \\ \vdots & \vdots & \vdots & & \vdots \\ \pi_s & \pi_s' & \pi_s'' & \cdots & \pi_s^{(s)} \\ \vdots & \vdots & \vdots & & \vdots \\ \pi_{n-1} & \pi_{n-1}' & \pi_{n-1}'' & \cdots & \pi_{n-1}^{(s)} \\ \pi_n & \pi_n' & \pi_n'' & \cdots & \pi_n^{(s)} \end{bmatrix}, \quad \boldsymbol{\rho} = \begin{bmatrix} \pi_0 & 0 & 0 & \cdots & 0 \\ 0 & \pi_0 & 0 & \cdots & 0 \\ 0 & \pi_1 & 2\pi_1' & \cdots & 0 \\ \vdots & \vdots & \vdots & & \vdots \\ 0 & \pi_{s-1} & 2\pi_{s-1}' & \cdots & s\pi_{s-1}^{(s-1)} \\ \vdots & \vdots & \vdots & & \vdots \\ 0 & \pi_{n-2} & 2\pi_{n-2}' & \cdots & s\pi_{n-2}^{(s-1)} \\ 0 & \pi_{n-1} & 2\pi_{n-1}' & \cdots & s\pi_{n-1}^{(s-1)} \end{bmatrix},$$

and

$$\boldsymbol{L} = \begin{bmatrix} 1 & 0 & 0 & \cdots & 0 & 0 \\ \beta_0^0 - t & 1 & 0 & \cdots & 0 & 0 \\ \beta_1^1 & \beta_0^1 - t & 1 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & & \vdots & \vdots \\ \beta_{n-2}^{n-2} & \beta_{n-3}^{n-2} & \beta_{n-4}^{n-2} & \cdots & 1 & 0 \\ \beta_{n-1}^{n-1} & \beta_{n-2}^{n-1} & \beta_{n-3}^{n-1} & \cdots & \beta_0^{n-1} - t & 1 \end{bmatrix}.$$

We define the vector $\boldsymbol{u} = [u_0, u_1, \ldots, u_n]^{\mathrm{T}}$ by

$$\boldsymbol{L}^{\mathrm{T}}\boldsymbol{u} = \boldsymbol{c}, \quad \boldsymbol{c}^{\mathrm{T}} = [c_0, c_1, \ldots, c_n], \tag{2.5.18}$$

which is equivalent to the relations

$$\begin{aligned} u_n &= c_n, \\ u_k &= (t - \beta_0^k)u_{k+1} - \sum_{\ell=1}^{n-1-k} \beta_\ell^{k+\ell} u_{k+\ell+1} + c_k, \\ &\qquad\qquad k = n-1, n-2, \ldots, 0. \end{aligned} \tag{2.5.19}$$

Then,

$$\boldsymbol{c}^{\mathrm{T}}\boldsymbol{\pi}(t) = [r(t), r'(t), \ldots, r^{(s)}] \tag{2.5.20}$$

is the vector of the sum (2.5.16) and its first s derivatives. On the other hand, by (2.5.17) and (2.5.18), since $\pi_0 = 1$,

$$\begin{aligned} \boldsymbol{c}^{\mathrm{T}}\boldsymbol{\pi} &= \boldsymbol{c}^{\mathrm{T}}\boldsymbol{L}^{-1}\boldsymbol{\rho} = ((\boldsymbol{L}^{\mathrm{T}})^{-1}\boldsymbol{c})^{\mathrm{T}}\boldsymbol{\rho} = \boldsymbol{u}^{\mathrm{T}}\boldsymbol{\rho} \\ &= \left[u_0, \sum_{j=0}^{n-1} u_{j+1}\pi_j, 2\sum_{j=1}^{n-1} u_{j+1}\pi_j', \ldots, s\sum_{j=s-1}^{n-1} u_{j+1}\pi_j^{(s-1)} \right]. \end{aligned} \tag{2.5.21}$$

Thus, $r(t) = u_0$ can be computed by the algorithm (2.5.19). From (2.5.20) and (2.5.21) it is seen that $r'(t)$ is also a sum of the type (2.5.16), with leading coefficient equal to zero and the other coefficients c_j replaced by u_{j+1}. Thus, $r'(t)$ can be computed by the same algorithm (2.5.19) suitably modified. Now that we have an algorithm for $r'(t)$, we can use it, with appropriate modifications, to compute the next component in (2.5.21), and so on. This is implemented for the first two derivatives in the `OPQ` routine `clenshaw_sob.m`, which finds an application in §3.2.3, Example 3.53.

2.6 Notes to Chapter 2

§2.1.2. The condition numbers of functions and maps, as defined in this section, are widely adopted, explicitly or implicitly. See, for example, Gautschi (1984c), (1997b, Chapter 1, §3). The idea of a mollified condition number, though natural, appears to be new.

§2.1.3. The moment map $\boldsymbol{G}_n$ was introduced and studied as early as 1968 by Gautschi (1968). It has been further studied, along with the maps $\boldsymbol{K}_n$ and $\boldsymbol{H}_n$, in Gautschi (1982b).

§2.1.4. Theorem 2.11 is due to Gautschi (1968) (see also Gautschi (1982b, §3.2)). Example 2.12, slightly sharpened, is taken from Gautschi (1968). Theorem 2.13 is similar to ideas expressed in Gautschi (1982b, p. 301). Examples 2.14–2.16 are new.

§2.1.5. Theorem 2.17 is due to Gautschi (1982b, Theorem 3.1). So are the discussions regarding the computation of the function g_n (*ibid.*, p. 304).

§2.1.6. Theorem 2.22 and Examples 2.23–2.25 are due to Fischer (1996). The results of this section are used in Beckermann and Bourreau (1998) to derive upper and lower bounds for the condition number of $\boldsymbol{K}_n$.

§2.1.7. Algorithm 2.1, in the form given, is due to Wheeler (1974), and in a somewhat different form, to Sack and Donovan (1969), (1972). (Equation (3.4) in Wheeler (1974) is misprinted: a_k, b_k should read a_ℓ and b_ℓ, respectively.) The discretized version of the algorithm, described at the end of the section, is suggested in Gautschi (1981b, §5.3). A generalization of the modified Chebyshev algorithm to indefinite inner products is discussed in Golub and Gutknecht (1990) along with relevant matrix interpretations and an "inverse" Chebyshev algorithm. Modified moments relative to polynomials p_k satisfying an extended (not necessarily three-term) recurrence relation and the required modifications in the modified Chebyshev algorithm are considered in Gragg and Gutknecht (1994).

An analog of the modified Chebyshev algorithm for Szegö polynomials, including a study of the conditioning of the underlying map, is developed in Jagels and Reichel (1993). For an extension of the modified Chebyshev algorithm to matrix orthogonal polynomials, see Bourreau (2000).

§2.1.8.1. The original reference for Clenshaw's algorithm is Clenshaw (1955). The matrix interpretation of Algorithm 2.2 is taken from Deuflhard (1974). The algorithm is applicable also to nonpolynomial functions satisfying a three-term recurrence relation, but should be avoided for minimal solutions of such recurrence relations because of potentially large cancellation errors (Elliott, 1968). A more stable algorithm, in this case, is proposed in Deuflhard (1977). For other possible extensions, see Saffren and Ng (1971). There are Clenshaw-type algorithms also for derivatives of finite orthogonal series; see Smith (1965), Cooper (1967), and Hunter (1970). Error analyses of Clenshaw's algorithm can be found in Elliott (1968), Oliver (1977), Barrio (2002), and Smoktunowicz (2002), and implementations on parallel computers in Barrio (2000).

A Clenshaw-type algorithm for Szegö polynomials is developed in Ammar et al. (1993).

§2.1.8.2. An ingenious conversion algorithm, in part based on Clenshaw's algorithm, was already devised by Salzer (1973). Algorithm 2.4, proposed in Laurie (1997, §3), simplifies Salzer's algorithm at the expense of having to store a matrix of mixed moments.

For an algorithm converting a linear combination of Szegö polynomials into polynomial form, see Ammar et al. (1993).

§2.1.9. Example 2.26 was first considered, from the point of view of conditioning, in Gautschi (1982b, Example 4.1) and further discussed in Gautschi (1984c, Example 5.1). Note, however, that cond $\widetilde{\boldsymbol{G}}_n(\boldsymbol{m})$ in eqn (3.15) of Gautschi (1982b) is defined somewhat differently than in (2.1.50), containing an extra factor. Example 2.29 is also taken from Gautschi (1982b), and so is Example 2.27 for $\alpha = 0$.

The general case $\alpha > -1$ is treated in Gautschi (1984c, Example 5.3); see also Gautschi (1994, Example 3.2). Example 2.31 and the inadequacy of Hermite and Laguerre modified moments is pointed out in Gautschi (1982b, Example 4.6) and is further analyzed in Gautschi (1984c, Example 5.4). An important generalization involves the Hermite measure on the interval $[0, c]$, $0 < c \leq \infty$ (cf. Example 1.11), which is discussed in Gautschi (1990, pp. 196–197) and Gautschi (1991b, pp. 64–66). The latter reference, in particular, contains graphs of the polynomial g_n showing how instability develops as c is increased from $c = 0.5$ to $c = 5$. For this, see also Gautschi (1996, p. 86). For Hermite measures on finite intervals, see also Chin (1992).

Other notable measures for which the modified Chebyshev algorithm fails are singular measures supported on Cantor-like sets; see, in particular, Mantica (1996), and also Mantica (2000).

§2.2.1. Theorem 2.32 and its Corollary are given in Gautschi (1968, §4); it can also be obtained from a more general theorem of Kripke (1964) on best approximation with respect to nearby norms.

§2.2.2. The idea of discretizing inner products and, in particular, to use the Fejér quadrature rule for this purpose goes back to Gautschi (1968) and is further developed in Gautschi (1982b). The procedure proposed for partitioning an interval, and the related Examples 2.33 and 2.34, are new.

§2.2.3.1. The bootstrap procedure of generating the recurrence coefficients of discrete orthogonal polynomials, attributed to Stieltjes, has been developed and used independently by Forsythe (1957) in the context of data fitting. Example 2.35 is from Gautschi (1994, Example 4.1) and Example 2.36 from Gautschi (1982b, Example 4.2).

§2.2.3.2. Example 2.37 is from Gautschi (1982b, Example 4.1). For a variant and extension of the Gragg–Harrod algorithm, and comparison with Stieltjes's procedure, see Reichel (1993).

§2.2.4. Example 2.38 was first given in Gautschi (1982b, Example 4.9), following a suggestion by M. Golomb. The multiple-component discretization method, essentially as described in this subsection, was developed in Gautschi (1994, §4.3), and in a more rudimentary form already in Gautschi (1982b, §2.2).

§2.2.5. Example 2.39 is from Gautschi (1994, Example 4.3), where the data on errors have been replaced with comparisons between the Stieltjes and Lanczos algorithms. The application to generalized Jacobi measures was mentioned in Gautschi (1996, Example 6.2), but the numerical tests provided in Example 2.40 are new. Examples 2.41 and 2.44 are from Gautschi (1994, Examples 4.5 and 4.4), and Example 2.45 from Gautschi (1982b, Example 4.10), with the numerical examples given being new. A (partly empirical) nonlinear recurrence procedure for the recursion coefficients of the generalized half-range Hermite measure $t^{\alpha}\mathrm{e}^{-t^2}\,\mathrm{d}t$ on $[0, \infty]$ (cf. Example 2.41) has been developed recently by Ball (2003).

§2.2.6. The idea of using discretized modified moments in the modified Chebyshev algorithm was first advanced in Gautschi (1981b, §5.3). Example 2.46 is

from Gautschi (1982b, Example 4.6).

§2.3.1. Minimality of the Cauchy integrals $\rho_n(z)$ has been noted in Gautschi (1981a). The recursive computation of the integrals $\rho_n(x)$ is applied in Gautschi (1981b, §3.2.3) to compute Cauchy principal value integrals.

§2.3.2. The computation of Cauchy integrals by the continued fraction algorithm was proposed in Gautschi (1981a, §5). The algorithm itself, and underlying theory, goes back to Gautschi (1967a, §3).

§2.3.3. The application of Cauchy integrals to Gauss quadrature remainders and their estimates, given in Example 2.47, is the subject of Gautschi and Varga (1983) and Gautschi, Tychopoulos, and Varga (1990). Further advances on this topic can be found in Gautschi and Li (1990), Gautschi (1991d), Schira (1994), (1996), (1997), Scherer and Schira (2000), Hunter and Nikolov (2000), and Milovanović and Spalević (2003). The procedure described in Example 2.49 is from Gautschi (1981a, §4). The material in Examples 2.50 and 2.51 is original.

§2.4. Modification by a linear factor was originally considered by Galant (1971). A solution to all the other modifications discussed in this section was first given in Gautschi (1982a). Other approaches have been described in Kautský and Golub (1983) and Fischer and Golub (1992); see also Gautschi (2002, §3). The algorithms presented in this section are new and were motivated by work of Verlinden (1999), who considered linear and quadratic divisors. (The middle term in eqn (17) of Verlinden (1999) should be removed.)

§2.4.5. Algorithm 2.11 is new and supersedes an earlier algorithm derived in Gautschi (1999, §3.3) in connection with Gauss quadrature rules for rational functions. For other treatments of special quadratic divisors, see Berti and Sri Ranga (2001).

§2.4.6. Example 2.56 comes from Gautschi (1994, Example 5.2) and Examples 2.58 and 2.59 from Gautschi (1994, Example 5.3), except that actual errors are replaced by discrepancies between the results produced by the modified Chebyshev and the modification algorithms. Example 2.57 is new. Example 2.60 repeats the numerical example given in Gautschi (1982a, §6), but provides the exact answers to higher precision. Example 2.61 is new. Example 2.56 has been generalized by Li (1999), who considers modification of the measure $d\lambda$ by an arbitrary even power of π_m.

§2.5. The methods described in this section are discussed more completely in Gautschi and Zhang (1995), not only with regard to algorithmic details, but also with regard to numerical accuracy. For special classes of Sobolev inner products there are simpler recurrence relations of finite order; cf. the Notes to §1.7. An example of this is an inner product that involves one single derivative and a discrete one-point measure associated therewith; see Marcellán and Ronveaux (1990). Computational methods for these special Sobolev orthogonal polynomials are developed in Gautschi (1997c).

§2.5.1. Example 2.62 is from Gautschi and Zhang (1995, §3.1).

§2.5.3. Examples 2.63 and 2.64 are new.

§2.5.4. The material in this subsection is original.

3

APPLICATIONS

3.1 Quadrature

The connection between orthogonal polynomials and quadrature rules has already been elucidated in §1.4. The centerpieces were the Gaussian quadrature rule and its close relatives—the Gauss–Radau and Gauss–Lobatto rules (§1.4.2). There are, however, a number of further extensions of Gauss's approach to numerical quadrature. Principal among them are Kronrod's idea of extending an n-point Gauss rule to a $(2n+1)$-point rule by inserting $n+1$ additional nodes and choosing all weights in such a way as to maximize the degree of exactness (cf. Definition 1.44), and Turán's extension of the Gauss quadrature rule allowing not only function values, but also derivative values, to appear in the quadrature sum. More recent extensions relate to the concept of accuracy, requiring exactness not only for polynomials of a certain degree, but also for rational functions with prescribed poles. Gauss quadrature can also be adapted to deal with Cauchy principal value integrals, and there are other applications of Gauss's ideas, for example, in combination with Stieltjes's procedure or the modified Chebyshev algorithm, to generate polynomials orthogonal on several intervals, or, in comnbination with Lanczos's algorithm, to estimate matrix functionals. The present section is to discuss these questions in turn, with computational aspects foremost in our mind.

3.1.1 *Computation of Gauss-type quadrature formulae*

We have previously seen in Chapter 2 how Gauss quadrature rules can be effectively employed in the context of computational methods; for example, in computing the absolute and relative condition numbers of moment maps (§2.1.5), or as a means of discretizing measures in the multiple-component discretization method for orthogonal polynomials (§2.2.5) and in Stieltjes-type methods for Sobolev orthogonal polynomials (§2.5.2). It is time now to discuss the actual computation of these, and related, quadrature rules.

3.1.1.1 *Gauss quadrature formula* We begin with the Gauss quadrature formula (cf. (1.4.7)),

$$\int_{\mathbb{R}} f(t)\,\mathrm{d}\lambda(t) = \sum_{\nu=1}^{n} \lambda_\nu^G f(\tau_\nu^G) + R_n^G(f). \tag{3.1.1}$$

A clue towards computing it comes from the spectral decomposition of the Jacobi matrix $\boldsymbol{J}_n(\mathrm{d}\lambda)$ of the (positive) measure $\mathrm{d}\lambda$ (cf. Definition 1.30). We al-

ready know from Theorem 1.31 that the Gauss nodes $\tau_\nu^G = \tau_\nu^{(n)}$—the zeros of $\pi_n(\,\cdot\,;\mathrm{d}\lambda)$—are the eigenvalues of $\boldsymbol{J}_n(\mathrm{d}\lambda)$. With $\boldsymbol{v}_\nu$, as in (1.3.19), denoting the corresponding normalized eigenvectors, let $\boldsymbol{V} = [\boldsymbol{v}_1, \boldsymbol{v}_2, \ldots, \boldsymbol{v}_n]$, so that $\boldsymbol{V}$ is the orthogonal matrix effecting the spectral decomposition of $\boldsymbol{J} = \boldsymbol{J}_n(\mathrm{d}\lambda)$,

$$\boldsymbol{J}\boldsymbol{V} = \boldsymbol{V}\boldsymbol{D}_\tau, \quad \boldsymbol{D}_\tau = \mathrm{diag}(\tau_1^G, \tau_2^G, \ldots, \tau_n^G). \tag{3.1.2}$$

Theorem 3.1 *The nodes τ_ν^G, $\nu = 1, 2, \ldots, n$, of the n-point Gauss quadrature rule (3.1.1) are the eigenvalues of the Jacobi matrix $\boldsymbol{J}_n(\mathrm{d}\lambda)$, and the weights λ_ν^G, $\nu = 1, 2, \ldots, n$, are*

$$\lambda_\nu^G = \beta_0 \boldsymbol{v}_{\nu,1}^2, \tag{3.1.3}$$

where $\beta_0 = \int_{\mathbb{R}} \mathrm{d}\lambda(t)$ and $\boldsymbol{v}_{\nu,1}$ is the first component of the normalized eigenvector $\boldsymbol{v}_\nu$ belonging to the eigenvalue τ_ν^G.

Proof Let $\tilde\pi_k(t) = \tilde\pi_k(t;\mathrm{d}\lambda)$ be the orthonormal polynomials relative to the measure $\mathrm{d}\lambda$ and $\tilde{\boldsymbol{\pi}}(t) = [\tilde\pi_0(t), \tilde\pi_1(t), \ldots, \tilde\pi_{n-1}(t)]^{\mathrm{T}}$, as in (1.3.17), the vector of the first n of them. By Theorem 1.31 and its Corollary,

$$\beta_0 \boldsymbol{v}_{\nu,1}^2 = \frac{1}{\sum_{k=0}^{n-1} [\tilde\pi_k(\tau_\nu^G)]^2}, \quad \nu = 1, 2, \ldots, n. \tag{3.1.4}$$

On the other hand, letting $f(t) = \tilde\pi_k(t)$, $k \le n-1$, in the Gauss formula (3.1.1) and noting that $\tilde\pi_0 = \beta_0^{-1/2}$, one obtains by orthogonality,

$$\beta_0^{1/2}\delta_{k,0} = \sum_{\nu=1}^{n} \lambda_\nu^G \tilde\pi_k(\tau_\nu^G), \quad \delta_{k,0} \text{ the Kronecker delta},$$

or, in matrix form,

$$\boldsymbol{P}\boldsymbol{\lambda}^G = \beta_0^{1/2}\boldsymbol{e}_1, \tag{3.1.5}$$

where $\boldsymbol{P}$ is the matrix of eigenvectors and $\boldsymbol{\lambda}^G$ the vector of Gauss weights,

$$\boldsymbol{P} = [\tilde{\boldsymbol{\pi}}(\tau_1^G), \tilde{\boldsymbol{\pi}}(\tau_2^G), \ldots, \tilde{\boldsymbol{\pi}}(\tau_n^G)], \quad \boldsymbol{\lambda}^G = [\lambda_1^G, \lambda_2^G, \ldots, \lambda_n^G]^{\mathrm{T}}, \tag{3.1.6}$$

and $\boldsymbol{e}_1^{\mathrm{T}} = [1, 0, \ldots, 0] \in \mathbb{R}^n$ the first coordinate vector. Since the columns of $\boldsymbol{P}$ are mutually orthogonal, there holds

$$\boldsymbol{P}^{\mathrm{T}}\boldsymbol{P} = \boldsymbol{D}_\pi, \quad \boldsymbol{D}_\pi = \mathrm{diag}(d_0, d_1, \ldots, d_{n-1}), \quad d_{\nu-1} = \sum_{k=0}^{n-1} [\tilde\pi_k(\tau_\nu^G)]^2.$$

Multiplying (3.1.5) from the left by $\boldsymbol{P}^{\mathrm{T}}$, one gets

$$\boldsymbol{D}_\pi \boldsymbol{\lambda}^G = \beta_0^{1/2}\boldsymbol{P}^{\mathrm{T}}\boldsymbol{e}_1 = \beta_0^{1/2} \cdot \beta_0^{-1/2}\boldsymbol{e} = \boldsymbol{e},$$

where $\boldsymbol{e} = [1, 1, \ldots, 1]^{\mathrm{T}} \in \mathbb{R}^n$. There follows $\boldsymbol{\lambda}^G = \boldsymbol{D}_\pi^{-1}\boldsymbol{e}$, that is,

$$\lambda_\nu^G = \frac{1}{\sum_{k=0}^{n-1} [\tilde\pi_k(\tau_\nu^G)]^2}, \quad \nu = 1, 2, \ldots, n. \tag{3.1.7}$$

Assertion (3.1.3) now follows from (3.1.4). □

Theorem 3.1 is implemented in the `OPQ` routine `gauss.m`.

Remark to Theorem 3.1 If f is sufficiently smooth, for example analytic in an interval containing all the Gauss nodes τ_ν^G, then $f(\boldsymbol{J})$, $\boldsymbol{J} = \boldsymbol{J}_n(\mathrm{d}\lambda)$, is meaningful and the Gauss quadrature sum in (3.1.1) can be expressed as follows:

$$\sum_{\nu=1}^{n} \lambda_\nu^G f(\tau_\nu^G) = \beta_0 \boldsymbol{e}_1^{\mathrm{T}} f(\boldsymbol{J}) \boldsymbol{e}_1, \quad \boldsymbol{e}_1^{\mathrm{T}} = [1, 0, \ldots, 0] \in \mathbb{R}^n. \tag{3.1.8}$$

Indeed, using (3.1.2) and (3.1.3), one has

$$\beta_0 \boldsymbol{e}_1^{\mathrm{T}} f(\boldsymbol{J}) \boldsymbol{e}_1 = \beta_0 \boldsymbol{e}_1^{\mathrm{T}} \boldsymbol{V} f(\boldsymbol{D}_{\boldsymbol{\tau}}) \boldsymbol{V}^{\mathrm{T}} \boldsymbol{e}_1 = \beta_0 \sum_{\nu=1}^{n} \boldsymbol{v}_{\nu,1}^2 f(\tau_\nu^G) = \sum_{\nu=1}^{n} \lambda_\nu^G f(\tau_\nu^G).$$

Corollary to Theorem 3.1 Let $\boldsymbol{\lambda}^G$ be as in (3.1.6), and $\boldsymbol{D}_\tau$ as in (3.1.2). Then, there exists an orthogonal matrix $\boldsymbol{Q} \in \mathbb{R}^n$ such that

$$\begin{bmatrix} 1 & \boldsymbol{0}^{\mathrm{T}} \\ \boldsymbol{0} & \boldsymbol{Q}^{\mathrm{T}} \end{bmatrix} \begin{bmatrix} 1 & \sqrt{\boldsymbol{\lambda}^G}^{\mathrm{T}} \\ \sqrt{\boldsymbol{\lambda}^G} & \boldsymbol{D}_\tau \end{bmatrix} \begin{bmatrix} 1 & \boldsymbol{0}^{\mathrm{T}} \\ \boldsymbol{0} & \boldsymbol{Q} \end{bmatrix} = \begin{bmatrix} 1 & \sqrt{\beta_0} \boldsymbol{e}_1^{\mathrm{T}} \\ \sqrt{\beta_0} \boldsymbol{e}_1 & \boldsymbol{J}_n(\mathrm{d}\lambda) \end{bmatrix}. \tag{3.1.9}$$

The matrix on the right may be thought of as an "extended" Jacobi matrix of the measure $\mathrm{d}\lambda$.

Proof We claim that $\boldsymbol{Q} = \boldsymbol{V}^{\mathrm{T}}$. In order to see this, we write (3.1.3) in matrix form as

$$\sqrt{\boldsymbol{\lambda}}^{\mathrm{T}} = \sqrt{\beta_0} \boldsymbol{e}_1^{\mathrm{T}} \boldsymbol{V}, \quad \sqrt{\boldsymbol{\lambda}} = \left[\sqrt{\lambda_1^G}, \sqrt{\lambda_2^G}, \ldots, \sqrt{\lambda_n^G} \right]^{\mathrm{T}}, \tag{3.1.10}$$

where the first components of the normalized eigenvectors are assumed to be positive. We now combine (3.1.10) (after transposing the first relation) with (3.1.2) to obtain

$$\boldsymbol{V} \boldsymbol{D}_\tau \boldsymbol{V}^{\mathrm{T}} = \boldsymbol{J}, \quad \boldsymbol{V} \sqrt{\boldsymbol{\lambda}} = \sqrt{\beta_0} \boldsymbol{e}_1.$$

Thus,

$$\begin{bmatrix} 1 & \boldsymbol{0}^{\mathrm{T}} \\ \boldsymbol{0} & \boldsymbol{V} \end{bmatrix} \begin{bmatrix} 1 & \sqrt{\boldsymbol{\lambda}}^{\mathrm{T}} \\ \sqrt{\boldsymbol{\lambda}} & \boldsymbol{D}_\tau \end{bmatrix} \begin{bmatrix} 1 & \boldsymbol{0}^{\mathrm{T}} \\ \boldsymbol{0} & \boldsymbol{V}^{\mathrm{T}} \end{bmatrix} = \begin{bmatrix} 1 & \sqrt{\boldsymbol{\lambda}}^{\mathrm{T}} \boldsymbol{V}^{\mathrm{T}} \\ \boldsymbol{V} \sqrt{\boldsymbol{\lambda}} & \boldsymbol{V} \boldsymbol{D}_\tau \boldsymbol{V}^{\mathrm{T}} \end{bmatrix} = \begin{bmatrix} 1 & \sqrt{\beta_0} \boldsymbol{e}_1^{\mathrm{T}} \\ \sqrt{\beta_0} \boldsymbol{e}_1 & \boldsymbol{J} \end{bmatrix},$$

which proves (3.1.9) with $\boldsymbol{Q} = \boldsymbol{V}^{\mathrm{T}}$. □

We make two observations: (1) The orthogonal similarity transformation (3.1.9) suggests, though not necessarily proves,[3] that the passage from the Gauss

[3]See, however, Theorem 1 and Corollary 8 in Beckermann and Bourreau (1998) or the theorem on p. 168 of Laurie (1999a).

quantities (more precisely, the n square roots $\sqrt{\lambda_\nu^G}$ and n nodes τ_ν^G) to the recursion coefficients (more precisely, the $2n$ quantities $\sqrt{\beta_\nu}$, α_ν in $\boldsymbol{J}_n(\mathrm{d}\lambda)$) is a stable process. (2) If $\mathrm{d}\lambda = \mathrm{d}\lambda_N$ is a discrete measure with N support points t_k and positive weights w_k, then by definition

$$\int_{\mathbb{R}} p(t)\,\mathrm{d}\lambda_N(t) = \sum_{k=1}^{N} w_k p(t_k). \tag{3.1.11}$$

In particular, this holds for any polynomial p of degree $\leq 2N-1$. The sum on the right, therefore, may be interpreted as the N-point Gauss formula for the measure $\mathrm{d}\lambda_N$. If $\sqrt{\boldsymbol{w}}^{\mathrm{T}} = [\sqrt{w_1}, \sqrt{w_2}, \ldots, \sqrt{w_N}\,]$ and $\boldsymbol{D}_t = \mathrm{diag}(t_1, t_2, \ldots, t_N)$, we have by (3.1.9),

$$\begin{bmatrix} 1 & \boldsymbol{0}^{\mathrm{T}} \\ \boldsymbol{0} & \boldsymbol{Q}^{\mathrm{T}} \end{bmatrix} \begin{bmatrix} 1 & \sqrt{\boldsymbol{w}}^{\mathrm{T}} \\ \sqrt{\boldsymbol{w}} & \boldsymbol{D}_t \end{bmatrix} \begin{bmatrix} 1 & \boldsymbol{0}^{\mathrm{T}} \\ \boldsymbol{0} & \boldsymbol{Q} \end{bmatrix} = \begin{bmatrix} 1 & \sqrt{\beta_{0,N}}\boldsymbol{e}_1^{\mathrm{T}} \\ \sqrt{\beta_{0,N}}\boldsymbol{e}_1 & \boldsymbol{J}_N(\mathrm{d}\lambda_N) \end{bmatrix} \tag{3.1.12}$$

for some orthogonal matrix $\boldsymbol{Q} \in \mathbb{R}^N$. This provides the basis for a Lanczos-type algorithm computing the extended Jacobi matrix of a discrete measure $\mathrm{d}\lambda_N$ from the weights w_k and abscissae t_k of the measure (cf. §2.2.3.2).

3.1.1.2 *Gauss–Radau formula* We recall from §1.4.2, eqn (1.4.21), that the $(n+1)$-point Gauss–Radau quadrature rule, having $a = \inf \mathrm{supp}(\mathrm{d}\lambda)$ as a fixed node, is given by

$$\int_{\mathbb{R}} f(t)\,\mathrm{d}\lambda(t) = \lambda_0^a f(\tau_0^a) + \sum_{\nu=1}^{n} \lambda_\nu^a f(\tau_\nu^a) + R_n^a(f). \tag{3.1.13}$$

Here, $\tau_0^a = a$, and τ_ν^a are the zeros of $\pi_n(\,\cdot\,;\mathrm{d}\lambda_a)$, where $\mathrm{d}\lambda_a(t) = (t-a)\,\mathrm{d}\lambda(t)$. An eigenvalue/eigenvector characterization similar to the one in Theorem 3.1 holds also for the Gauss–Radau formula.

Theorem 3.2 *Define the* Jacobi–Radau matrix *of order* $n+1$ *by*

$$\boldsymbol{J}_{n+1}^{R,a}(\mathrm{d}\lambda) = \begin{bmatrix} \boldsymbol{J}_n(\mathrm{d}\lambda) & \sqrt{\beta_n}\boldsymbol{e}_n \\ \sqrt{\beta_n}\boldsymbol{e}_n^{\mathrm{T}} & \alpha_n^R \end{bmatrix}, \quad \boldsymbol{e}_n^{\mathrm{T}} = [0, 0, \ldots, 1] \in \mathbb{R}^n, \tag{3.1.14}$$
$$\alpha_n^R = a - \beta_n \frac{\pi_{n-1}(a)}{\pi_n(a)},$$

where $\beta_n = \beta_n(\mathrm{d}\lambda)$ *and* $\pi_m(\,\cdot\,) = \pi_m(\,\cdot\,;\mathrm{d}\lambda)$. *Then, the nodes* $\tau_0^a\,(=a), \tau_1^a, \ldots, \tau_n^a$ *of the Gauss–Radau formula (3.1.13) are the eigenvalues of* $\boldsymbol{J}_{n+1}^{R,a}(\mathrm{d}\lambda)$, *and the weights* $\lambda_0^a, \lambda_1^a, \ldots, \lambda_n^a$ *are*

$$\lambda_\nu^a = \beta_0 \boldsymbol{v}_{\nu,1}^2, \quad \nu = 0, 1, 2, \ldots, n, \tag{3.1.15}$$

where $\beta_0 = \int_{\mathbb{R}} \mathrm{d}\lambda(t)$ *and* $\boldsymbol{v}_{\nu,1}$ *is the first component of the normalized eigenvector* $\boldsymbol{v}_\nu$ *of* $\boldsymbol{J}_{n+1}^{R,a}(\mathrm{d}\lambda)$ *corresponding to the eigenvalue* τ_ν^a.

Proof As in the proof of Theorem 3.1, let $\tilde{\pi}_k$ denote the orthonormal polynomials relative to the measure $\mathrm{d}\lambda$, and let $\tilde{\boldsymbol{\pi}}(t) = [\tilde{\pi}_0(t), \tilde{\pi}_1(t), \ldots, \tilde{\pi}_n(t)]^{\mathrm{T}}$ be the vector of the first $n+1$ of them. Recall from Theorem 1.29 that

$$t\tilde{\pi}_k(t) = \alpha_k \tilde{\pi}_k(t) + \sqrt{\beta_k}\tilde{\pi}_{k-1}(t) + \sqrt{\beta_{k+1}}\tilde{\pi}_{k+1}(t), \quad k = 0, 1, 2, \ldots, n-1, \tag{3.1.16}$$

to which we now adjoin the additional relation

$$t\tilde{\pi}_n(t) = \alpha_n^R \tilde{\pi}_n(t) + \sqrt{\beta_n}\tilde{\pi}_{n-1}(t) + \sqrt{\beta_{n+1}}\pi_{n+1}^R(t). \tag{3.1.17}$$

Here, $\beta_{n+1} = \beta_{n+1}(\mathrm{d}\lambda)$, and α_n^R for the moment is a parameter to be determined; once α_n^R is known, eqn (3.1.17) defines π_{n+1}^R. Written in matrix form, (3.1.16) and (3.1.17) yield

$$t\tilde{\boldsymbol{\pi}}(t) = \boldsymbol{J}_{n+1}^{R,a}\tilde{\boldsymbol{\pi}}(t) + \sqrt{\beta_{n+1}}\pi_{n+1}^R(t)\boldsymbol{e}_{n+1}, \quad \boldsymbol{e}_{n+1}^{\mathrm{T}} = [0, 0, \ldots, 1] \in \mathbb{R}^{n+1}, \tag{3.1.18}$$

where $\boldsymbol{J}_{n+1}^{R,a} = \boldsymbol{J}_{n+1}^{R,a}(\mathrm{d}\lambda)$. We now choose α_n^R in such a way that $\pi_{n+1}^R(a) = 0$, so that $\tau_0^a = a$ is an eigenvalue of $\boldsymbol{J}_{n+1}^{R,a}$ (with $\tilde{\boldsymbol{\pi}}(a)$ a corresponding eigenvector) and (3.1.17) gives

$$a\tilde{\pi}_n(a) - \alpha_n^R \tilde{\pi}_n(a) - \sqrt{\beta_n}\tilde{\pi}_{n-1}(a) = 0.$$

Solving for α_n^R and reverting to monic orthogonal polynomials, noting that $\tilde{\pi}_{n-1}/\tilde{\pi}_n = \sqrt{\beta_n}\pi_{n-1}/\pi_n$, yields the formula for α_n^R in (3.1.14). Since (by construction) a is a zero of π_{n+1}^R, we can write

$$\pi_{n+1}^R(t) = (t-a)\omega_n(t), \quad \omega_n \in \mathbb{P}_n. \tag{3.1.19}$$

The zeros t_ν, $\nu = 1, 2, \ldots, n$, of ω_n, by (3.1.18), all are eigenvalues of $\boldsymbol{J}_{n+1}^{R,a}$, with $\tilde{\boldsymbol{\pi}}(t_\nu)$ corresponding eigenvectors. We now show that $t_\nu = \tau_\nu^a$—the internal nodes of the Gauss–Radau formula (3.1.13). For this, we must show that, up to a constant factor,

$$\omega_n(t) = \pi_n(t; \mathrm{d}\lambda_a),$$

or, by (3.1.19), equivalently,

$$\int_{\mathbb{R}} \pi_{n+1}^R(t) p(t)\, \mathrm{d}\lambda(t) = 0 \quad \text{for all } p \in \mathbb{P}_{n-1}.$$

This follows by (3.1.17), which implies

$$\begin{aligned}
&\sqrt{\beta_{n+1}} \int_{\mathbb{R}} \pi_{n+1}^R(t) p(t)\, \mathrm{d}\lambda(t) \\
&\quad = \int_{\mathbb{R}} [(t-\alpha_n^R)\tilde{\pi}_n(t) - \sqrt{\beta_n}\tilde{\pi}_{n-1}(t)] p(t)\, \mathrm{d}\lambda(t) \\
&\quad = \int_{\mathbb{R}} [(t-\alpha_n+\alpha_n-\alpha_n^R)\tilde{\pi}_n(t) - \sqrt{\beta_n}\tilde{\pi}_{n-1}(t)] p(t)\, \mathrm{d}\lambda(t) \\
&\quad = \int_{\mathbb{R}} [\sqrt{\beta_{n+1}}\tilde{\pi}_{n+1}(t) + (\alpha_n-\alpha_n^R)\tilde{\pi}_n(t)] p(t)\, \mathrm{d}\lambda(t) \\
&\quad = 0
\end{aligned}$$

by orthogonality. This proves the first part of the theorem.

The second part follows along the same lines as in the proof of Theorem 3.1, noting that the normalized eigenvectors $\boldsymbol{v}_\nu$, $\nu = 0, 1, \ldots, n$, of $\boldsymbol{J}_{n+1}^{R,a}$ are

$$\boldsymbol{v}_\nu = \left(\sum_{k=0}^{n} [\tilde{\pi}_k(\tau_\nu^a)]^2 \right)^{-1/2} \tilde{\boldsymbol{\pi}}(\tau_\nu^a), \quad \nu = 0, 1, 2, \ldots, n,$$

and, hence, by comparing the first component on each side and squaring,

$$\beta_0 \boldsymbol{v}_{\nu,1}^2 = \frac{1}{\sum_{k=0}^{n} [\tilde{\pi}_k(\tau_\nu^a)]^2}, \quad \nu = 0, 1, 2, \ldots, n \tag{3.1.20}$$

(cf. Corollary to Theorem 1.31). The rest of the proof is virtually identical with the proof of Theorem 3.1. □

Theorem 3.2 is implemented in the `OPQ` routine `radau.m`.

Remarks to Theorem 3.2 (a) Theorem 3.2 remains valid if $a < \inf \operatorname{supp}(\mathrm{d}\lambda)$.

(b) If $\operatorname{supp}(\mathrm{d}\lambda)$ is bounded from above, there is an analogous Gauss–Radau formula

$$\int_{\mathbb{R}} f(t)\, \mathrm{d}\lambda(t) = \sum_{\nu=1}^{n} \lambda_\nu^b f(\tau_\nu^b) + \lambda_{n+1}^b f(\tau_{n+1}^b) + R_n^b(f), \quad b \geq \sup \operatorname{supp}(\mathrm{d}\lambda), \tag{3.1.21}$$

for which Theorem 3.2 again holds with a replaced by b throughout, and $\tau_0^a = a$, λ_0^a replaced, respectively, by $\tau_{n+1}^b = b$, λ_{n+1}^b. The internal nodes τ_ν^b are the zeros of $\pi_n(\,\cdot\,; \mathrm{d}\lambda_b)$, where $\mathrm{d}\lambda_b(t) = (b-t)\, \mathrm{d}\lambda(t)$.

(c) For smooth f, the Gauss–Radau quadrature sum in (3.1.13), similarly as in Remark to Theorem 3.1, can be expressed in matrix form as $\beta_0 \boldsymbol{e}_1^{\mathrm{T}} f(\boldsymbol{J}_{n+1}^{R,a}) \boldsymbol{e}_1$.

Theorem 3.3 *If the support of* $\mathrm{d}\lambda$ *is a finite interval* $[a, b]$ *and* $f \in C^{2n+1}[a, b]$, *then the remainders* R_n^a, R_n^b *in (3.1.13) resp. (3.1.21) have the property*

$$R_n^a(f) > 0, \quad R_n^b(f) < 0 \quad \textit{if } \operatorname{sgn} f^{(2n+1)} = 1 \textit{ on } [a, b], \tag{3.1.22}$$

with the inequalities reversed if $\operatorname{sgn} f^{(2n+1)} = -1$.

Thus, one of the Gauss–Radau approximants is a lower bound, and the other an upper bound for the exact value of the integral.

Proof This follows from the formula (cf. (1.4.23))

$$R_n^a(f) = \gamma_n^a \frac{f^{(2n+1)}(\tau^a)}{(2n+1)!}, \quad \gamma_n^a = \int_a^b [\pi_n(t; \mathrm{d}\lambda_a)]^2 \, \mathrm{d}\lambda_a(t), \quad a < \tau^a < b,$$

and the analogous formula for R_n^b,

$$R_n^b(f) = -\gamma_n^b \frac{f^{(2n+1)}(\tau^b)}{(2n+1)!}, \quad \gamma^b = \int_a^b [\pi_n(t; \mathrm{d}\lambda_b)]^2 \, \mathrm{d}\lambda_b(t), \quad a < \tau^b < b.$$

(The minus sign in R_n^b comes from changing the factor $t - b$ in the node polynomial to $b - t$ to make it, and with it $\mathrm{d}\lambda_b(t) = (b-t)\,\mathrm{d}\lambda(t)$, positive on $[a, b]$.) □

Example 3.4 Gauss–Radau formula for the Jacobi measure.

Here, $\mathrm{d}\lambda$ is the Jacobi measure $\mathrm{d}\lambda^{(\alpha,\beta)}(t) = (1-t)^\alpha (1+t)^\beta \, \mathrm{d}t$ on $[-1, 1]$. In this case, the quantity α_n^R, $n \geq 1$, in the Jacobi–Radau matrix (3.1.14) can be expressed explicitly in terms of the Jacobi parameters α, β,

$$\alpha_n^R = \begin{cases} -1 + \dfrac{2n(n+\alpha)}{(2n+\alpha+\beta)(2n+\alpha+\beta+1)} & \text{if } a = -1, \\ 1 - \dfrac{2n(n+\beta)}{(2n+\alpha+\beta)(2n+\alpha+\beta+1)} & \text{if } a = 1. \end{cases} \tag{3.1.23}$$

To see this, let $\pi_k = \pi_k^{(\alpha,\beta)}$ denote the monic Jacobi polynomials and $P_k = P_k^{(\alpha,\beta)}$ the Jacobi polynomials as conventionally defined. Then (cf. Commentary to Table 1.1),

$$P_n(t) = k_n \pi_n(t), \quad k_n = \frac{1}{2^n} \binom{2n+\alpha+\beta}{n}, \quad P_n(-1) = (-1)^n \binom{n+\beta}{n}.$$

Therefore, in the case $a = -1$, by (3.1.14),

$$\alpha_n^R = -1 - \beta_n \frac{\pi_{n-1}(-1)}{\pi_n(-1)} = -1 - \beta_n \frac{k_n}{k_{n-1}} \frac{P_{n-1}(-1)}{P_n(-1)}. \tag{3.1.24}$$

A simple computation shows that

$$\frac{k_n}{k_{n-1}} = \frac{1}{2} \frac{(2n+\alpha+\beta)(2n+\alpha+\beta-1)}{n(n+\alpha+\beta)}, \quad \frac{P_{n-1}(-1)}{P_n(-1)} = -\frac{n}{n+\beta}.$$

Substituting this in (3.1.24) and using the expression for $\beta_n = \beta_n^J$ from Table 1.1 yields the first relation in (3.1.23). The second is obtained analogously.

For a Matlab implementation, see the `OPQ` routine `radau_jacobi.m`. Explicit expressions are also known for all the weights in the Gauss–Radau formula, obviating the need to compute eigenvectors; see Gautschi (2000a, §3 and 4).

Example 3.5 Gauss–Radau formula for the generalized Laguerre measure.

Here, the measure is $\mathrm{d}\lambda^{(\alpha)}(t) = t^{\alpha}\mathrm{e}^{-t}\,\mathrm{d}t$ on $[0,\infty]$, $\alpha > -1$, and the explicit formula for α_n^R turns out to be particularly simple,

$$\alpha_n^R = n \quad \text{if } a = 0. \tag{3.1.25}$$

Indeed, with $\pi_k^{(\alpha)}$ and $L_k^{(\alpha)}$ denoting the monic resp. conventional Laguerre polynomials, there holds (cf. Commentary to Table 1.1)

$$L_n^{(\alpha)}(t) = \frac{(-1)^n}{n!}\,\pi_n^{(\alpha)}(t), \quad L_n^{(\alpha)}(0) = \binom{n+a}{n},$$

from which

$$\alpha_n^R = -\beta_n\,\frac{\pi_{n-1}^{(\alpha)}(0)}{\pi_n^{(\alpha)}(0)} = \beta_n\,\frac{L_{n-1}^{(\alpha)}(0)}{nL_n^{(\alpha)}(0)} = n(n+\alpha)\cdot\frac{1}{n+\alpha} = n,$$

since $\beta_n = n(n+\alpha)$ (cf. Table 1.1).

Example 3.5 is implemented in the `OPQ` routine `radau_laguerre.m`. Explicit formulae for the weights in the Gauss–Radau rule are provided in Gautschi (2000b, §5).

3.1.1.3 *Gauss–Lobatto formula* For measures $\mathrm{d}\lambda$ with finite support interval $[a,b]$, the $(n+2)$-point Gauss–Lobatto quadrature rule is (cf. §1.4.2, eqn (1.4.22))

$$\int_a^b f(t)\,\mathrm{d}\lambda(t) = \lambda_0^L f(\tau_0^L) + \sum_{\nu=1}^{n}\lambda_\nu^L f(\tau_\nu^L) + \lambda_{n+1}^L f(\tau_{n+1}^L) + R_n^{a,b}(f), \tag{3.1.26}$$

where $\tau_0^L = a$, $\tau_{n+1}^L = b$, and the internal nodes τ_ν^L are the zeros of $\pi_n(\,\cdot\,;\mathrm{d}\lambda_{a,b})$ with $\mathrm{d}\lambda_{a,b}(t) = (t-a)(b-t)\,\mathrm{d}\lambda(t)$. The Gauss–Lobatto formula enjoys an eigenvalue/vector characterization similar to the ones in Theorems 3.1 and 3.2.

Theorem 3.6 *Define the* Jacobi–Lobatto matrix *of order* $n+2$ *by*

$$\boldsymbol{J}_{n+2}^L(\mathrm{d}\lambda) = \begin{bmatrix} \boldsymbol{J}_{n+1}(\mathrm{d}\lambda) & \sqrt{\beta_{n+1}^L}\,\boldsymbol{e}_{n+1} \\ \sqrt{\beta_{n+1}^L}\,\boldsymbol{e}_{n+1}^{\mathrm{T}} & \alpha_{n+1}^L \end{bmatrix}, \quad \boldsymbol{e}_{n+1}^{\mathrm{T}} = [0,0,\ldots,1] \in \mathbb{R}^{n+1}, \tag{3.1.27}$$

where α_{n+1}^L, β_{n+1}^L *solve the* 2×2 *linear system*

$$\begin{bmatrix} \pi_{n+1}(a) & \pi_n(a) \\ \pi_{n+1}(b) & \pi_n(b) \end{bmatrix}\begin{bmatrix} \alpha_{n+1}^L \\ \beta_{n+1}^L \end{bmatrix} = \begin{bmatrix} a\pi_{n+1}(a) \\ b\pi_{n+1}(b) \end{bmatrix} \tag{3.1.28}$$

with $\pi_m(\,\cdot\,) = \pi_m(\,\cdot\,;\mathrm{d}\lambda)$. *Then, the nodes* $\tau_0^L\,(=a), \tau_1^L, \ldots, \tau_n^L, \tau_{n+1}^L\,(=b)$ *of the Gauss–Lobatto formula (3.1.26) are the eigenvalues of* $\boldsymbol{J}_{n+2}^L(\mathrm{d}\lambda)$, *and the weights* $\lambda_0^L, \lambda_1^L, \ldots, \lambda_n^L, \lambda_{n+1}^L$ *are*

$$\lambda_\nu^L = \beta_0 \boldsymbol{v}_{\nu,1}^2, \quad \nu = 0, 1, \ldots, n, n+1, \tag{3.1.29}$$

where $\beta_0 = \int_a^b \mathrm{d}\lambda(t)$ *and* $\boldsymbol{v}_{\nu,1}$ *is the first component of the normalized eigenvector* $\boldsymbol{v}_\nu$ *of* $\boldsymbol{J}_{n+2}^L(\mathrm{d}\lambda)$ *corresponding to the eigenvalue* τ_ν^L.

Proof The recurrence relations (3.1.16) for the orthonormal polynomials are now adjoined by two additional relations,

$$\begin{aligned} t\tilde{\pi}_n(t) &= \alpha_n \tilde{\pi}_n(t) + \sqrt{\beta_n}\tilde{\pi}_{n-1}(t) + \sqrt{\beta_{n+1}^L}\pi_{n+1}^L(t), \\ t\pi_{n+1}^L(t) &= \alpha_{n+1}^L \pi_{n+1}^L(t) + \sqrt{\beta_{n+1}^L}\tilde{\pi}_n(t) + \sqrt{\beta_{n+2}}\pi_{n+2}^L(t), \end{aligned} \tag{3.1.30}$$

where, for the moment, α_{n+1}^L and β_{n+1}^L are parameters to be determined, and $\alpha_n = \alpha_n(\mathrm{d}\lambda)$, $\beta_n = \beta_n(\mathrm{d}\lambda)$, $\beta_{n+2} = \beta_{n+2}(\mathrm{d}\lambda)$. Once the parameters α_{n+1}^L and β_{n+1}^L have been assigned real values, with $\beta_{n+1}^L > 0$, the first relation in (3.1.30) defines π_{n+1}^L, and the second π_{n+2}^L, both as real polynomials. Relations (3.1.16) and (3.1.30) together can be written in matrix form,

$$t\tilde{\boldsymbol{\pi}}(t) = \boldsymbol{J}_{n+2}^L \tilde{\boldsymbol{\pi}}(t) + \sqrt{\beta_{n+2}}\pi_{n+2}^L(t)\boldsymbol{e}_{n+2}, \tag{3.1.31}$$

where $\boldsymbol{J}_{n+2}^L = \boldsymbol{J}_{n+2}^L(\mathrm{d}\lambda)$ and $\tilde{\boldsymbol{\pi}}(t) = [\tilde{\pi}_0(t), \ldots, \tilde{\pi}_n(t), \pi_{n+1}^L(t)]^{\mathrm{T}}$. The parameters α_{n+1}^L, β_{n+1}^L are now chosen so as to have $\pi_{n+2}^L(a) = \pi_{n+2}^L(b) = 0$, which by (3.1.31) means that a and b are both eigenvalues of $\boldsymbol{J}_{n+2}^L$ (with $\tilde{\boldsymbol{\pi}}(a)$ and $\tilde{\boldsymbol{\pi}}(b)$ corresponding eigenvectors). By the second relation of (3.1.30), this requires

$$(t - \alpha_{n+1}^L)\pi_{n+1}^L(t) - \sqrt{\beta_{n+1}^L}\tilde{\pi}_n(t) = 0 \quad \text{for } t = a, b,$$

or, multiplying by $\sqrt{\beta_{n+1}^L}$ and substituting $\sqrt{\beta_{n+1}^L}\pi_{n+1}^L(t)$ from the first relation of (3.1.30),

$$(t - \alpha_{n+1}^L)[(t - \alpha_n)\tilde{\pi}_n(t) - \sqrt{\beta_n}\tilde{\pi}_{n-1}(t)] - \beta_{n+1}^L \tilde{\pi}_n(t) = 0 \quad \text{for } t = a, b.$$

The expression in brackets is $\sqrt{\beta_{n+1}}\tilde{\pi}_{n+1}(t)$, so that

$$(t - \alpha_{n+1}^L)\sqrt{\beta_{n+1}}\tilde{\pi}_{n+1}(t) - \beta_{n+1}^L \tilde{\pi}_n(t) = 0 \quad \text{for } t = a, b.$$

Converting this to monic orthogonal polynomials yields the system (3.1.28).

We must check that β_{n+1}^L so determined is positive. This follows from

$$[\pi_{n+1}(a)\pi_n(b) - \pi_{n+1}(b)\pi_n(a)]\beta_{n+1}^L = (b - a)\pi_{n+1}(a)\pi_{n+1}(b),$$

since the expression in brackets—the determinant of the system (3.1.28)—has the sign $(-1)^{n+1}$ and so does the right-hand side.

Since (by construction) a and b are zeros of π_{n+2}^L, we can write

$$\pi_{n+2}^L(t) = (t-a)(b-t)\omega_n(t), \quad \omega_n \in \mathbb{P}_n. \tag{3.1.32}$$

The zeros t_ν, $\nu = 1, 2, \ldots, n$, of ω_n, by (3.1.31), all are eigenvalues of $\boldsymbol{J}_{n+2}^L$, with $\tilde{\boldsymbol{\pi}}(t_\nu)$ corresponding eigenvectors. We show that they are precisely the internal nodes τ_ν^L of the Gauss–Lobatto formula (3.1.26). For this, we must show that, up to a constant factor,

$$\omega_n(t) = \pi_n(t; \mathrm{d}\lambda_{a,b}),$$

or, by (3.1.32),

$$\int_a^b \pi_{n+2}^L(t) p(t)\, \mathrm{d}\lambda(t) = 0 \quad \text{for all } p \in \mathbb{P}_{n-1}.$$

This follows from (3.1.30), which implies

$$\begin{aligned}
&\sqrt{\beta_{n+1}^L \beta_{n+2}} \int_a^b \pi_{n+2}^L(t) p(t)\, \mathrm{d}\lambda(t) \\
&\quad = \sqrt{\beta_{n+1}^L} \int_a^b [(t-\alpha_{n+1}^L)\pi_{n+1}^L(t) - \sqrt{\beta_{n+1}^L}\tilde{\pi}_n(t)] p(t)\, \mathrm{d}\lambda(t) \\
&\quad = \int_a^b \{(t-\alpha_{n+1}^L)[(t-\alpha_n)\tilde{\pi}_n(t) - \sqrt{\beta_n}\tilde{\pi}_{n-1}(t)] - \beta_{n+1}^L \tilde{\pi}_n(t)\} p(t)\, \mathrm{d}\lambda(t) \\
&\quad = \int_a^b [(t-\alpha_{n+1}^L)\sqrt{\beta_{n+1}}\tilde{\pi}_{n+1}(t) - \beta_{n+1}^L \tilde{\pi}_n(t)] p(t)\, \mathrm{d}\lambda(t) \\
&\quad = 0
\end{aligned}$$

by orthogonality. This proves the first part of the theorem. The second part follows in the same manner as in the proof of Theorem 3.2, by letting f in the Gauss–Lobatto formula be in turn $\tilde{\pi}_0, \tilde{\pi}_1, \ldots, \tilde{\pi}_n$, and π_{n+1}^L. □

Theorem 3.6 is implemented in the `OPQ` routine `lobatto.m`.

Remarks to Theorem 3.6 (a) Theorem 3.6 remains valid if $\tau_0^L < a$ and/or $\tau_{n+1}^L > b$, provided a and/or b in (3.1.28) are replaced, respectively, by τ_0^L and τ_{n+1}^L.

(b) As in Remark to Theorem 3.1, for smooth f the Gauss–Lobatto quadrature sum in (3.1.26) can be expressed in matrix form as $\beta_0 \boldsymbol{e}_1^{\mathrm{T}} f(\boldsymbol{J}_{n+2}^L)\boldsymbol{e}_1$.

Theorem 3.7 *If $f \in C^{2n+2}[a,b]$, the remainder $R_n^{a,b}$ in (3.1.26) has the property*

$$R_n^{a,b}(f) < 0 \quad \textit{if } \operatorname{sgn} f^{(2n+2)} = 1 \textit{ on } [a,b], \tag{3.1.33}$$

with the inequality reversed if $\operatorname{sgn} f^{(2n+2)} = -1$.

Proof This is an immediate consequence of (1.4.24). □

Example 3.8 Gauss–Lobatto formula for the Jacobi measure.

For the Jacobi measure $\mathrm{d}\lambda = \mathrm{d}\lambda^{(\alpha,\beta)}$ on $[-1,1]$, the quantities α_{n+1}^L and β_{n+1}^L can be expressed explicitly in terms of the Jacobi parameters α and β,

$$\begin{aligned} \alpha_{n+1}^L &= \frac{\alpha-\beta}{2n+\alpha+\beta+2}\,, \\ \beta_{n+1}^L &= 4\,\frac{(n+\alpha+1)(n+\beta+1)(n+\alpha+\beta+1)}{(2n+\alpha+\beta+1)(2n+\alpha+\beta+2)^2}\,. \end{aligned} \tag{3.1.34}$$

In fact, with notations used in Example 3.4, the determinant Δ_n of system (3.1.28) (where $a=-1$, $b=1$) is

$$\Delta_n = \frac{1}{k_n k_{n+1}}\, D_n,$$

where

$$D_n = \begin{vmatrix} P_{n+1}(-1) & P_n(-1) \\ P_{n+1}(1) & P_n(1) \end{vmatrix}.$$

Using the formula for $P_n(-1)$ in Example 3.4 and the companion formula $P_n(1) = \binom{n+\alpha}{n}$, one finds

$$D_n = \frac{(-1)^{n+1}}{n+1}\,(2n+\alpha+\beta+2)\binom{n+\alpha}{n}\binom{n+\beta}{n}.$$

Writing the solution of system (3.1.28) in the form

$$\begin{aligned} \alpha_{n+1}^L &= \frac{1}{D_n}\,[-P_{n+1}(-1)P_n(1) - P_{n+1}(1)P_n(-1)], \\ \beta_{n+1}^L &= \frac{2k_n}{k_{n+1}}\,\frac{1}{D_n}\,[P_{n+1}(-1)P_{n+1}(1)], \end{aligned}$$

and inserting the explicit expressions for the quantities appearing on the right-hand side yields (3.1.34).

Explicit expressions are also known for the weights in the Gauss–Lobatto formula; see Gautschi (2000b, §3 and 4).

When n is very large, the determinant Δ_n of system (3.1.28) may be so small as to underflow on a computer, causing the system to become numerically singular. In this event, the use of (3.1.34) is imperative. The respective `OPQ` routine is `lobatto_jacobi.m`.

3.1.1.4 *Generalized Gauss–Radau and Gauss–Lobatto formulae* It is sometimes useful, for example in the context of boundary value problems, to have at disposal Gauss-type quadrature rules that involve not only function values, but

also derivative values, at the end point(s). These are referred to as *generalized Gauss–Radau* resp. *Gauss–Lobatto formulae*.

We begin with the former, and consider

$$\int_a^\infty f(t)\,\mathrm{d}\lambda(t) = \sum_{\rho=0}^{r-1} \lambda_0^{(\rho)} f^{(\rho)}(a) + \sum_{\nu=1}^{n} \lambda_\nu^R f(\tau_\nu^R) + R_{n,r}^R(f), \tag{3.1.35}$$

where $r > 1$ is the multiplicity of the end point $\tau_0 = a$ and the degree of exactness is $2n - 1 + r$,

$$R_{n,r}^R(f) = 0 \quad \text{for all } f \in \mathbb{P}_{2n-1+r}. \tag{3.1.36}$$

The support of $\mathrm{d}\lambda$ may, or may not, be bounded. The internal nodes and weights are easily obtained according to the following theorem.

Theorem 3.9 *Let* $\mathrm{d}\lambda^{[r]}(t) = (t-a)^r\,\mathrm{d}\lambda(t)$ *and* $\tau_\nu^{[r]}$, $\lambda_\nu^{[r]}$, $\nu = 1, 2, \ldots, n$, *be the Gauss nodes and weights for the measure* $\mathrm{d}\lambda^{[r]}$. *Then,*

$$\tau_\nu^R = \tau_\nu^{[r]}, \quad \lambda_\nu^R = \frac{\lambda_\nu^{[r]}}{(\tau_\nu^R - a)^r}, \quad \nu = 1, 2, \ldots, n. \tag{3.1.37}$$

In particular, all λ_ν^R *are positive; if* $r = 2$, *the same is true for* λ_0 *and* λ_0'.

Proof If $g \in \mathbb{P}_{2n-1}$, formula (3.1.35) is exact for $f(t) = (t-a)^r g(t)$. There follows

$$\int_a^\infty g(t)\,\mathrm{d}\lambda^{[r]}(t) = \sum_{\nu=1}^{n} \lambda_\nu^R (\tau_\nu^R - a)^r \cdot g(\tau_\nu^R) \quad \text{for all } g \in \mathbb{P}_{2n-1},$$

proving (3.1.37). The positivity of the weights λ_ν^R is a consequence of the positivity of $\mathrm{d}\lambda^{[r]}$ and the fact that $\tau_\nu^R > a$. If $r = 2$, putting in turn $f(t) = \pi_n^2(t)$ and $f(t) = (t-a)\pi_n^2(t)$, where $\pi_n(t) = \prod_{\nu=1}^n (t - \tau_\nu^R)$, yields

$$\pi_n^2(a)\lambda_0 + 2\pi_n(a)\pi_n'(a)\lambda_0' = \int_a^\infty \pi_n^2(t)\,\mathrm{d}\lambda(t),$$
$$\pi_n^2(a)\lambda_0' = \int_a^\infty (t-a)\pi_n^2(t)\,\mathrm{d}\lambda(t),$$

from which the positivity of λ_0 and λ_0' follows by virtue of the right-hand sides being positive and $\pi_n(a)\pi_n'(a) < 0$. □

In general, the boundary weights $\lambda_0^{(\rho)}$ have to be obtained by solving a linear system of equations, for example, the upper triangular system that obtains by applying (3.1.35) in turn for $\pi_n(t), (t-a)\pi_n(t), \ldots, (t-a)^{r-1}\pi_n(t)$, where π_n is as defined in the proof of Theorem 3.9.

Example 3.10 Gauss–Radau formula with double end points for the Legendre measure.

The measure here is $\mathrm{d}\lambda(t) = \mathrm{d}t$ on $[-1,1]$, and the formula in question is

$$\int_{-1}^{1} f(t)\,\mathrm{d}t = \lambda_0 f(-1) + \lambda_0' f'(-1) + \sum_{\nu=1}^{n} \lambda_\nu^R f(\tau_\nu^R) + R_{n,2}^R(f),$$

where τ_ν^R and λ_ν^R are the Gauss nodes and weights for $\mathrm{d}\lambda^{[2]}(t) = (1+t)^2\,\mathrm{d}t$. The boundary weights are given by

$$\lambda_0 = \frac{8}{3}\,\frac{2n^2+6n+3}{(n+1)^2(n+2)^2}\,, \quad \lambda_0' = \frac{8}{(n+1)^2(n+2)^2}\,.$$

This can be seen by inserting $f(t) = P_n^{(0,2)}(t)$ and $f(t) = (1+t)P_n^{(0,2)}(t)$ into the quadrature rule and solving the two linear equations thus obtained for λ_0 and λ_0'. For the values of $P_n^{(0,2)}(-1)$ and $(\mathrm{d}/\mathrm{d}t)P_n^{(0,2)}(-1) = \frac{1}{2}(n+3)P_{n-1}^{(1,3)}(-1)$, see the Commentaries to Table 1.1, and Erdélyi, Magnus, Oberhettinger, and Tricomi (1954, 16.4(1), p. 284) for the integrals $\int_{-1}^{1} P_n^{(0,2)}(t)\,\mathrm{d}t$, $\int_{-1}^{1}(1+t)P_n^{(0,2)}(t)\,\mathrm{d}t$.

Example 3.11 Gauss–Radau formula with double end points for the Chebyshev measure.

Here,

$$\int_{-1}^{1} f(t)(1-t^2)^{-1/2}\,\mathrm{d}t = \lambda_0 f(-1) + \lambda_0' f'(-1) + \sum_{\nu=1}^{n} \lambda_\nu^R f(\tau_\nu^R) + R_{n,2}^R(f),$$

where τ_ν^R and λ_ν^R are the Gauss nodes and weights for the Jacobi weight function $(1-t)^{-1/2}(1+t)^{3/2}$. The boundary weights are given by (Gautschi and Li, 1991, Theorem 2.3)

$$\lambda_0 = \frac{3}{5}\,\pi\frac{6n^2+12n+5}{(n+1)(2n+1)(2n+3)}\,, \quad \lambda_0' = \frac{3\pi}{(n+1)(2n+1)(2n+3)}\,.$$

We write the generalized Gauss–Lobatto formula in the form

$$\int_a^b f(t)\,\mathrm{d}\lambda(t) = \sum_{\rho=0}^{r-1} \lambda_0^{(\rho)} f^{(\rho)}(a) + \sum_{\nu=1}^{n} \lambda_\nu^L f(\tau_\nu^L) + \sum_{\rho=0}^{r-1} (-1)^\rho \lambda_{n+1}^{(\rho)} f^{(\rho)}(b) + R_{n,r}^L(f) \tag{3.1.38}$$

to reflect its symmetry $\lambda_0^{(\rho)} = \lambda_{n+1}^{(\rho)}$, $\rho = 0, 1, \ldots, r-1$, when $\mathrm{d}\lambda$ is a symmetric measure (cf. Definition 1.16). There holds $R_{n,r}^L(f) = 0$ if $f \in \mathbb{P}_{2n-1+2r}$.

Theorem 3.12 *Let* $\mathrm{d}\lambda^{[r]}(t) = [(t-a)(b-t)]^r\,\mathrm{d}\lambda(t)$ *and* $\tau_\nu^{[r]}$, $\lambda_\nu^{[r]}$, $\nu = 1, 2, \ldots, n$, *be the Gauss nodes and weights for the measure* $\mathrm{d}\lambda^{[r]}$. *Then,*

$$\tau_\nu^L = \tau_\nu^{[r]}, \quad \lambda_\nu^L = \frac{\lambda_\nu^{[r]}}{[(\tau_\nu^L - a)(b-\tau_\nu^L)]^r}\,, \quad \nu = 1, 2, \ldots, n.$$

In particular, all λ_ν^L *are positive; if* $r = 2$, *the same is true for* λ_0, λ_0' *and* λ_{n+1}, λ_{n+1}'.

Proof Similar to the proof of Theorem 3.9. The last statement for $r = 2$ with regard to λ_0 and λ_0' follows by inserting in succession $f(t) = \pi_n^2(t)(b-t)^2$ and $(t-a)\pi_n^2(t)(b-t)^2$ into (3.1.38) and noting that $\pi_n(a)(b-a)[\pi_n'(a)(b-a)-\pi_n(a)] < 0$. Similarly for λ_{n+1}, λ_{n+1}'. □

Example 3.13 Gauss–Lobatto formula with double end points for the Legendre measure.

Similarly as in Example 3.10 (or see Gatteschi (1964)), one derives

$$\int_{-1}^{1} f(t)\,\mathrm{d}t = \lambda_0[f(-1)+f(1)] + \lambda_0'[f'(-1)-f'(1)] + \sum_{\nu=1}^{n} \lambda_\nu^L f(\tau_\nu^L) + R_{n,2}^L(f)$$

with τ_ν^L and λ_ν^L the Gauss nodes and weights for the Gegenbauer weight function $(1-t^2)^2$ and

$$\lambda_0 = \frac{8}{3}\,\frac{2n^2+10n+9}{(n+1)(n+2)(n+3)(n+4)}, \quad \lambda_0' = \frac{8}{(n+1)(n+2)(n+3)(n+4)}.$$

Example 3.14 Gauss–Lobatto formula with double end points for the Chebyshev measure.

Here,

$$\int_{-1}^{1} f(t)(1-t^2)^{-1/2}\,\mathrm{d}t = \lambda_0[f(-1)+f(1)]+\lambda_0'[f'(-1)-f'(1)]+\sum_{\nu=1}^{n} \lambda_\nu^L f(\tau_\nu^L)+R_{n,2}^L(f),$$

where τ_ν^L and λ_ν^L are the Gauss nodes and weights for the Gegenbauer weight function $(1-t^2)^{3/2}$. The boundary weights are (Gautschi and Li, 1991, Theorem 3.3)

$$\lambda_0 = \frac{3}{10}\,\pi\,\frac{3n^2+12n+10}{(n+1)(n+2)(n+3)}, \quad \lambda_0' = \frac{3\pi}{4(n+1)(n+2)(n+3)}.$$

3.1.2 *Gauss–Kronrod quadrature formulae and their computation*

3.1.2.1 *Gauss–Kronrod formula* Given an n-point Gauss quadrature rule (3.1.1), one may wish to extend it to a $(2n+1)$-point rule by inserting $n+1$ additional nodes—preferably all in the support interval of $\mathrm{d}\lambda$ and alternating with the Gauss nodes—and choosing them, together with all weights, in such a manner as to achieve maximum degree of exactness (cf. Definition 1.44). This is an idea that was first put forward and implemented (in the case $\mathrm{d}\lambda(t) = \mathrm{d}t$) by Kronrod in the mid-1960s (Kronrod, 1965). His motivation was to estimate the error in the Gauss formula, using the result of the extended formula as a reference value for the integral. The point is that the n function values already computed for the Gauss formula are being reused, and only $n+1$ additional function values need to be computed to perform the error estimation. This is the same amount of work that an $(n+1)$-point Gauss formula would entail, but the

latter would produce a reference value much less accurate, in general, than the one produced by the extended $(2n+1)$-point formula.

The extended formula, thus, has the form

$$\int_{\mathbb{R}} f(t)\,\mathrm{d}\lambda(t) = \sum_{\nu=1}^{n} \lambda_\nu^K f(\tau_\nu^G) + \sum_{\mu=1}^{n+1} \lambda_\mu^{*K} f(\tau_\mu^K) + R_n^K(f), \tag{3.1.39}$$

where τ_ν^G are the Gauss nodes in (3.1.1), and all weights λ_ν^K, λ_μ^{*K} as well as the new nodes τ_μ^K are parameters that can be freely chosen. Since there are $3n+2$ of them, one can expect to be able to choose them so as to yield a degree of exactness as high as $3n+1$,

$$R_n^K(f) = 0 \quad \text{for all } f \in \mathbb{P}_{3n+1}. \tag{3.1.40}$$

A quadrature rule (3.1.39) satisfying (3.1.40) is called a *Gauss–Kronrod formula*, and the nodes τ_μ^K are referred to as *Kronrod nodes*.

In the terminology of §1.4.1, where n has to be replaced by $2n+1$, the node polynomial of (3.1.39) is

$$\omega_{2n+1}(t) = \pi_n(t;\mathrm{d}\lambda)\pi_{n+1}^K(t), \quad \pi_{n+1}^K(t) = \prod_{\mu=1}^{n+1}(t-\tau_\mu^K), \tag{3.1.41}$$

and by Theorem 1.45, in order to have (3.1.40) (which corresponds to $k = n+1$ in Theorem 1.45), it must satisfy $\int_{\mathbb{R}} \omega_{2n+1}(t)p(t)\,\mathrm{d}\lambda(t) = 0$ for all polynomials of degree $\leq n$, that is,

$$\int_{\mathbb{R}} \pi_{n+1}^K(t)p(t)\pi_n(t;\mathrm{d}\lambda)\,\mathrm{d}\lambda(t) = 0 \quad \text{for all } p \in \mathbb{P}_n. \tag{3.1.42}$$

This is a condition on the Kronrod nodes; once they are determined and none of them coincides with a Gauss node, the weights in (3.1.39) then follow from the interpolatory nature of (3.1.39), that is, from the fact that $R_n^K(f) = 0$ for all $f \in \mathbb{P}_{2n}$.

Condition (3.1.42) is a new type of orthogonality: it requires the polynomial π_{n+1}^K of degree $n+1$ to be orthogonal to all polynomials of lower degree relative to the measure $\mathrm{d}\lambda_n^K(t) = \pi_n(t;\mathrm{d}\lambda)\,\mathrm{d}\lambda(t)$, which not only depends on n but is also oscillating on the support of $\mathrm{d}\lambda$. Historically, such polynomials (in the case of $\mathrm{d}\lambda(t) = \mathrm{d}t$) were first considered in 1894 by Stieltjes in his last letter to Hermite (Baillaud and Bourget, 1905, Vol. II, p. 439). The polynomial $\pi_{n+1}^K(\,\cdot\,) = \pi_{n+1}^K(\,\cdot\,;\mathrm{d}\lambda)$, therefore, is nowadays referred to as the *Stieltjes polynomial* of degree $n+1$ relative to the measure $\mathrm{d}\lambda$.

Theorem 3.15 *If* $\mathrm{d}\lambda$ *is a positive measure, the Stieltjes polynomial* $\pi_{n+1}^K(\,\cdot\,;\mathrm{d}\lambda)$ *exists uniquely for each* $n \geq 1$.

Proof If we write $\pi_{n+1}^K(t) = t^{n+1} + \sum_{k=0}^n c_k t^k$, condition (3.1.42) takes the form

$$\int_{\mathbb{R}} \left(t^{n+\ell+1} + \sum_{k=0}^{n} c_k t^{k+\ell} \right) \pi_n(t)\, \mathrm{d}\lambda(t) = 0, \quad \ell = 0, 1, \ldots, n,$$

which is a linear system for the coefficients c_k whose matrix, by orthogonality, has nonzero elements only in its right lower triangle, those on the upward diagonal being $\int_{\mathbb{R}} t^n \pi_n(t)\, \mathrm{d}\lambda(t) = \|\pi_n\|_{\mathrm{d}\lambda}^2 > 0$. Therefore, the system is nonsingular. □

Although the unique existence of the Stieltjes polynomial is assured, it is by no means clear, and in fact often not the case, that its zeros—the Kronrod nodes—are all real, let alone contained in the support interval of $\mathrm{d}\lambda$ and interlacing with the Gauss nodes.

Example 3.16 Gauss–Kronrod formula for the Chebyshev measure $\mathrm{d}\lambda(t) = (1-t^2)^{-1/2}\, \mathrm{d}t$.

It turns out that this is precisely the Gauss–Lobatto formula (1.4.25) in which n is replaced by $2n-1$, that is, for $n \geq 2$,

$$\int_{-1}^{1} f(t)(1-t^2)^{-1/2}\, \mathrm{d}t = \frac{\pi}{4n}\left[f(-1) + f(1)\right] + \frac{\pi}{2n} \sum_{\nu=1}^{2n-1} f\left(\cos\frac{\nu\pi}{2n}\right) + R_n^K(f). \tag{3.1.43}$$

Indeed, the n nodes in the summation corresponding to odd values of ν are the Gauss nodes for $\mathrm{d}\lambda$ (cf. Example 1.49), and since (3.1.43) has degree of exactness $4n-1$ ($\geq 3n+1$), the remaining nodes must be the Kronrod nodes.

There are similar explicit formulae of elevated degree for all the other three Chebyshev measures; see Mysovskih (1964).

The Gauss–Kronrod formula of Example 3.16 is atypical for two reasons: first, there are two nodes on the boundary of $[-1, 1]$, and second, its degree of exactness exceeds the one normally expected for a Gauss–Kronrod rule. More typical, in this regard, are the Gauss–Kronrod formulae for the Gegenbauer measure $\mathrm{d}\lambda^{(\alpha,\alpha)}(t) = (1-t^2)^\alpha\, \mathrm{d}t$ when $-\frac{1}{2} < \alpha \leq \frac{3}{2}$. In this case, and hence in particular in the case $\alpha = 0$ originally considered by Kronrod, it has been shown by Szegö (1935) that all nodes are strictly inside the interval $[-1, 1]$ and the Kronrod nodes alternate with the Gauss nodes. Rabinowitz (1980) proved that the degree of exactness is precisely $3n+1$ (for n even, and $3n+2$ for n odd, by symmetry) except when $\alpha = \frac{1}{2}$, in which case it is $4n+1$. Moreover, Monegato (1978a) has shown that all weights are positive if $-\frac{1}{2} \leq \alpha \leq \frac{1}{2}$. For results and conjectures in the case $\frac{3}{2} < \alpha \leq \frac{5}{2}$, see Petras (1999) and Peherstorfer and Petras (2000), where nonexistence of Gauss–Kronrod formulae is shown for n sufficiently large and $\alpha > \frac{5}{2}$. Analogous results for the Jacobi measure $\mathrm{d}\lambda^{(\alpha,\beta)}(t) = (1-t)^\alpha(1+t)^\beta\, \mathrm{d}t$ can be found in Peherstorfer and Petras (2003), in particular nonexistence for large n of Gauss–Kronrod formulae when $\min(\alpha, \beta) \geq 0$ and $\max(\alpha, \beta) > \frac{5}{2}$. The case of Gegenbauer measures, and also of Jacobi measures, has been further

explored for $n \leq 40$ by numerical means with regard to interlacing, reality and containment in the open support interval of the Kronrod nodes, and positivity of the weights; see Gautschi and Notaris (1988). Classical measures on an infinite interval fare less well. Kahaner and Monegato (1978), in fact, show that for the generalized Laguerre measure $\mathrm{d}\lambda^{(\alpha)}(t) = t^{\alpha}\mathrm{e}^{-t}\,\mathrm{d}t$ on $[0,\infty]$, with $-1 < \alpha \leq 1$, a Kronrod extension of the Gauss–Laguerre formula having real nodes and positive weights does not exist when $n \geq 23$ and, if $\alpha = 0$, not even for $n > 1$. As a corollary of this, an n-point Gauss–Hermite formula cannot be so extended unless $n = 1, 2$, or 4.

3.1.2.2 *Computation of the Gauss–Kronrod formula* We sketch a computational algorithm due to Laurie; for more details, see Laurie (1997). We assume that a Gauss–Kronrod formula exists with real nodes and positive weights. The idea is to obtain an eigenvalue/vector characterization of the Gauss–Kronrod formula similar to the ones derived in §3.1.1.1–3.1.1.3 for Gauss-type quadrature rules. The matrix in question—now called the *Jacobi–Kronrod matrix*—is a Jacobi matrix of order $2n+1$ (cf. Definition 1.30), $\boldsymbol{J}^K_{2n+1}$, with coefficients $\alpha^K_0, \beta^K_1, \alpha^K_1, \beta^K_2, \ldots, \beta^K_{2n}$. The Gauss–Kronrod formula having degree of exactness $3n+1$ implies that the first $3n+1$ of these coefficients are those relative to the measure $\mathrm{d}\lambda$, that is, $\alpha_0, \beta_1, \alpha_1, \beta_2, \ldots$, where $\alpha_k = \alpha_k(\mathrm{d}\lambda)$, $\beta_k = \beta_k(\mathrm{d}\lambda)$. This means that $\boldsymbol{J}^K_{2n+1}$ has the form

$$\boldsymbol{J}^K_{2n+1}(\mathrm{d}\lambda) = \begin{bmatrix} \boldsymbol{J}_n(\mathrm{d}\lambda) & \sqrt{\beta_n}\,\boldsymbol{e}_n & \boldsymbol{0} \\ \sqrt{\beta_n}\,\boldsymbol{e}_n^{\mathrm{T}} & \alpha_n & \sqrt{\beta_{n+1}}\,\boldsymbol{e}_1^{\mathrm{T}} \\ \boldsymbol{0} & \sqrt{\beta_{n+1}}\,\boldsymbol{e}_1 & \boldsymbol{J}^*_n \end{bmatrix}, \tag{3.1.44}$$

where $\boldsymbol{e}_k$ denotes the kth coordinate vector in $\mathbb{R}^n$, and $\boldsymbol{J}^*_n$ is a real symmetric tridiagonal matrix whose form depends on the parity of n,

$$\boldsymbol{J}^*_n = \begin{bmatrix} \boldsymbol{J}_{n+1:(3n-1)/2}(\mathrm{d}\lambda) & \sqrt{\beta_{(3n+1)/2}}\,\boldsymbol{e}_{(n-1)/2} \\ \sqrt{\beta_{(3n+1)/2}}\,\boldsymbol{e}^{\mathrm{T}}_{(n-1)/2} & \boldsymbol{J}^*_{(3n+1)/2:2n} \end{bmatrix} \quad (n \text{ odd}), \tag{3.1.45}$$

$$\boldsymbol{J}^*_n = \begin{bmatrix} \boldsymbol{J}_{n+1:3n/2}(\mathrm{d}\lambda) & \sqrt{\beta^*_{(3n+2)/2}}\,\boldsymbol{e}_{n/2} \\ \sqrt{\beta^*_{(3n+2)/2}}\,\boldsymbol{e}^{\mathrm{T}}_{n/2} & \boldsymbol{J}^*_{(3n+2)/2:2n} \end{bmatrix} \quad (n \text{ even}). \tag{3.1.46}$$

Here, $\boldsymbol{J}_{p:q}(\mathrm{d}\lambda)$ is the principal minor matrix of the (infinite) Jacobi matrix $\boldsymbol{J}(\mathrm{d}\lambda)$ having diagonal elements $\alpha_p, \alpha_{p+1}, \ldots, \alpha_q$. The parameter $\beta^*_{(3n+2)/2}$ when n is

even, and the (real symmetric tridiagonal) matrices in the right lower corner of $\boldsymbol{J}_n^*$, are to be determined.

The following lemma is crucial for the algorithm.

Lemma 3.17 *The matrices $\boldsymbol{J}_n^*$ and $\boldsymbol{J}_n(\mathrm{d}\lambda)$ in (3.1.44) have the same eigenvalues.*

Proof Let $\phi_k(t)$ and $\psi_k(t)$ be the (monic) characteristic polynomials of the leading, respectively trailing, $k \times k$ principal minor matrix of $\boldsymbol{J}_{2n+1}^K$. Evidently, $\phi_k(t) = \pi_k(t; \mathrm{d}\lambda)$ when $k \leq n+1$. Expanding $\phi_{2n+1}(t) = \det(t\boldsymbol{I}_{2n+1} - \boldsymbol{J}_{2n+1}^K)$ along the $(n+1)$st row, one finds, after some computation, that

$$\phi_{2n+1}(t) = \beta_n \pi_{n-1}(t)\psi_n(t) + (t - \alpha_n)\pi_n(t)\psi_n(t) + \beta_{n+1}\pi_n(t)\psi_{n-1}(t). \quad (3.1.47)$$

Since the Gauss nodes τ_ν^G—the zeros of π_n—are to be eigenvalues of $\boldsymbol{J}_{2n+1}^K$, the polynomial π_n must be a factor of ϕ_{2n+1}, and hence, by (3.1.47), since $\beta_n > 0$, a factor of $\pi_{n-1}\psi_n$. By Theorem 1.20, the zeros of π_{n-1}, however, alternate with those of π_n. There follows that π_n must be a factor of ψ_n. Both polynomials are monic of degree n. Consequently, $\pi_n \equiv \psi_n$. □

Remark According to a result of Monegato (1976), the positivity of all λ_μ^{*K} is equivalent to the reality of the Kronrod nodes and their interlacing with the Gauss nodes.

Once the Jacobi–Kronrod matrix has been determined, the Gauss–Kronrod formula is computed in terms of the eigenvalues and eigenvectors of $\boldsymbol{J}_{2n+1}^K$ in much the same way as the Gauss formula in Theorem 3.1. It suffices, therefore, to compute the unknown elements in $\boldsymbol{J}_{2n+1}^K$; the recursion coefficients $\alpha_k(\mathrm{d}\lambda)$ and $\beta_k(\mathrm{d}\lambda)$ are assumed to be known.

To conform with notation used in §2.1.7–2.1.8, we write

$$\boldsymbol{J}_n^* = \begin{bmatrix} \alpha_0^* & \sqrt{\beta_1^*} & & \mathbf{0} \\ \sqrt{\beta_1^*} & \alpha_1^* & \ddots & \\ & \ddots & \ddots & \sqrt{\beta_{n-1}^*} \\ \mathbf{0} & & \sqrt{\beta_{n-1}^*} & \alpha_{n-1}^* \end{bmatrix}. \quad (3.1.48)$$

We thus have two Jacobi matrices—$\boldsymbol{J}_n(\mathrm{d}\lambda)$ and $\boldsymbol{J}_n^*$—both of order n and having the same eigenvalues. Each of these matrices generates its own set of orthogonal polynomials, the former the polynomials $\pi_k(\,\cdot\,; \mathrm{d}\lambda)$, $k = 0, 1, \ldots, n$, orthogonal with respect to the measure $\mathrm{d}\lambda$, the latter polynomials π_k^*, $k = 0, 1, \ldots, n$, orthogonal with respect to some measure $\mathrm{d}\lambda^*$ (in general unknown). We are in a situation reminiscent to the one surrounding the modified Chebyshev algorithm in §2.1.7 and the conversion algorithm in §2.1.8.2, which suggests similar approaches here. In particular, we define mixed moments by

$$\sigma_{k\ell} = (\pi_k^*, \pi_\ell)_{\mathrm{d}\lambda^*}. \quad (3.1.49)$$

Although the measure $d\lambda^*$ is unknown, a few things about these moments are known. For example,

$$\sigma_{k\ell} = 0 \quad \text{if } \ell < k, \tag{3.1.50}$$

by the orthogonality of π_k^*, and also

$$\sigma_{kn} = 0 \quad \text{if } k < n, \tag{3.1.51}$$

again by orthogonality, since $\pi_n = \pi_n^*$ by Lemma 3.17. Now recall the recurrence relation (2.1.121), which in the present context reads

$$\sigma_{k,\ell+1} - \sigma_{k+1,\ell} - (\alpha_k^* - \alpha_\ell)\sigma_{k\ell} - \beta_k^*\sigma_{k-1,\ell} + \beta_\ell\sigma_{k,\ell-1} = 0. \tag{3.1.52}$$

Some of the coefficients α_k^* and β_k^* are known according to the structure of the matrices (3.1.45) and (3.1.46). Indeed, if for definiteness we assume n odd, then

$$\alpha_k^* = \alpha_{n+1+k} \text{ for } 0 \le k \le (n-3)/2, \quad \beta_k^* = \beta_{n+1+k} \text{ for } 0 \le k \le (n-1)/2. \tag{3.1.53}$$

Thus, similarly as in Algorithm 2.4, by solving (3.1.52) for $\sigma_{k,\ell+1}$, we can compute the entries $\sigma_{k\ell}$ in the triangular array indicated by black dots in Fig. 3.1 (drawn

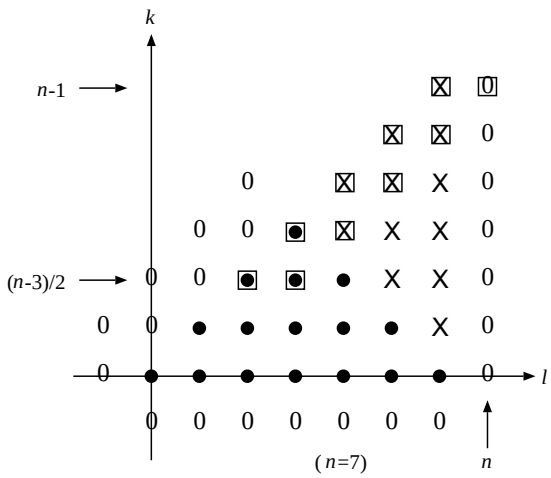

FIG. 3.1. Laurie's algorithm.

for $n = 7$), if we use the initialization $\sigma_{00} = \int_{\mathbb{R}} d\lambda^*(t) = \beta_0^* = \beta_{n+1}$, $\sigma_{-1,\ell} = 0$ for $\ell = 0, 1, \ldots, n-1$, $\sigma_{0,-1} = 0$, and $\sigma_{k,k-2} = \sigma_{k,k-1} = 0$ for $k = 1, 2, \ldots, (n-1)/2$. All the α_k^* and β_k^* required are, in fact, known by (3.1.53) except for the top element in the triangle. For this entry, the α_k^* for $k = (n-1)/2$ is not yet known, but by a stroke of good fortune, it multiplies the entry $\sigma_{(n-1)/2,(n-3)/2}$ in (3.1.52), which is zero by (3.1.50).

At this point, one switches to a recursion from bottom up, using the recursion (3.1.52) solved for $\sigma_{k+1,\ell}$. This computes all entries indicated by a cross in

Fig. 3.1, proceeding from the very bottom to the very top of the array. For this to be possible, it is crucial to have, by (3.1.51), the known zero entries for $\ell = n$. For each k with $(n-1)/2 \le k \le n-1$, the entries in Fig. 3.1 surrounded by boxes are those used, as in Algorithm 2.1, to compute the as yet unknown α_k^* and β_k^* according to

$$\alpha_k^* = \alpha_k + \frac{\sigma_{k,k+1}}{\sigma_{kk}} - \frac{\sigma_{k-1,k}}{\sigma_{k-1,k-1}}, \quad \beta_k^* = \frac{\sigma_{kk}}{\sigma_{k-1,k-1}}. \tag{3.1.54}$$

The complexity of the algorithm is $O(n^2)$. If any of the β_k^* turns out to be nonpositive, this would be an indication that a real Gauss–Kronrod formula does not exist.

Laurie in Appendix A of Laurie (1997) gives a pseudocode of the algorithm and kindly communicated to the author a Matlab version, which is incorporated in the OPQ routine `r_kronrod.m`. The latter is used in the routine `kronrod.m` to generate the respective quadrature rules.

Example 3.18 Kronrod's original formulae.

These refer to $\mathrm{d}\lambda(t) = \mathrm{d}t$ on $[0,1]$. The Matlab script

```
ab=r_jacobi01(61);
for N=[5 10 25 40]
   xw=kronrod(N,ab)
end
```

computes them for $n = 5, 10, 25, 40$ and produces results that agree with those tabulated in Kronrod (1965) within an error of usually a few units, and maximally 13 units, in the 16th decimal place.

Example 3.19 Gauss–Kronrod formulae for logarithmic measures.

As was already observed in Caliò, Gautschi, and Marchetti (1986), the logarithmic measure $\mathrm{d}\lambda(t) = \ln(1/t)\,\mathrm{d}t$ on $[0,1]$ appears to admit satisfactory Gauss–Kronrod formulae for all n, that is, formulae with real Kronrod nodes in $(0,1)$ interlacing with the Gauss nodes, and with positive weights. The Matlab script

```
ab=r_jaclog(39);
for N=5:5:25
   xw=kronrod(N,ab)
end
```

computes them for $n = 5, 10, 15, 20, 25$. Comparison with results in Caliò et al. (1986, S57–S63), obtained by Newton's method, reveals a level of agreement only slightly inferior to the one observed in Example 3.18, the maximum error now being 27 units in the 16th decimal place.

Exploring the more general logarithmic measure $\mathrm{d}\lambda^{(\alpha)}(t) = t^\alpha \ln(1/t)\,\mathrm{d}t$, we found for $\alpha > 0$ that there seems to exist an integer-valued function $n_0(\alpha)$ such that for $n < n_0(\alpha)$ a real, and in fact satisfactory, Gauss–Kronrod extension exists, but not so when $n = n_0(\alpha)$. Figure 3.2 shows a graph of the function $n_0(\alpha)$ experimentally determined by the OPQ routine `Example3_19.m`. The graph

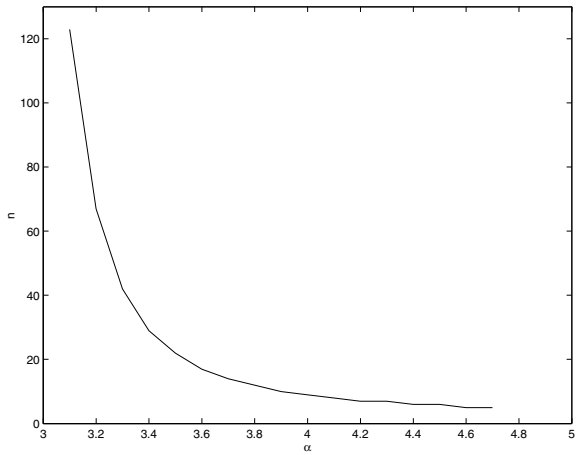

FIG. 3.2. The function $n_0(\alpha)$.

suggests that there might be a vertical asymptote at some $\alpha \geq 0$, so that the conjecture expressed at the beginning of the example is, in fact, true.

In the range $-1 < \alpha < 0$, a new phenomenon appears: when $n = 2$, there exists an α_0 in $(-1, 0)$ such that $\beta_4^* > 0$ for $\alpha_0 < \alpha < 0$ and $\beta_4^* < 0$ for $-1 < \alpha < \alpha_0$. In the latter case, a real Gauss–Kronrod formula, therefore, does not exist if $n = 2$. It was determined, numerically, that $-0.71417 < \alpha_0 < -0.71416$. As α moves further toward -1, more and more *even* values of n give rise to nonreal Gauss–Kronrod formulae. When real formulae exist—and that seems to be the case for all odd values of n—it was found (at least when $\alpha \geq -0.99$ and $n \leq 150$) that the Kronrod nodes interlace with the Gauss nodes and are < 1, and all weights are positive. The only defect observed was that initially, when n is odd, and eventually for all n that admit real formulae, the smallest Kronrod node is negative (though small in absolute value).

3.1.3 *Gauss–Turán quadrature formulae and their computation*

3.1.3.1 *Gauss–Turán formula* Turán (1950) was the first to apply Gauss's principle to quadrature formulae involving derivatives, that is, multiple nodes. We assume here that each node has the same multiplicity $r \geq 1$, so that

$$\int_{\mathbb{R}} f(t)\,\mathrm{d}\lambda(t) = \sum_{\nu=1}^{n} [\lambda_\nu f(\tau_\nu) + \lambda'_\nu f'(\tau_\nu) + \cdots + \lambda_\nu^{(r-1)} f^{(r-1)}(\tau_\nu)] + R_n(f). \quad (3.1.55)$$

The interpolation process underlying this formula is now Hermite interpolation, which, given any set of distinct nodes τ_ν, will yield degree of exactness $d = rn - 1$ for (3.1.55). The formula is, therefore, called *interpolatory* if $R_n(f) = 0$ for all $f \in \mathbb{P}_{rn-1}$. The theory of interpolatory quadrature formulae, expressed in Theorem 1.45 for ordinary quadrature rules, easily extends to the case of quadrature rules with multiple nodes (replace ω_n in §1.4.1 by ω_n^r). As a result, formula (3.1.55)

has degree of exactness $d = rn - 1 + k$ $(0 \le k \le n)$ *if and only if* (3.1.55) *is interpolatory and*

$$\int_{\mathbb{R}} \omega_n^r(t) p(t)\, \mathrm{d}\lambda(t) = 0 \quad \textit{for all } p \in \mathbb{P}_{k-1}, \tag{3.1.56}$$

where $\omega_n(t) = \prod_{\nu=1}^n (t - \tau_\nu)$ *is the node polynomial of* (3.1.55). Thus, it is now the rth power of ω_n, not ω_n, which must be orthogonal to all polynomials of degree $\le k-1$. This is referred to as *power orthogonality* (cf. also §1.2.4). Unless $k = 0$, the integer r must be odd, since otherwise $\int_{\mathbb{R}} \omega_n^r(t)\, \mathrm{d}\lambda(t) > 0$, and ω_n^r cannot be orthogonal to a constant, let alone to $\mathbb{P}_{k-1}$. We assume, therefore,

$$r = 2s + 1, \quad s \ge 0, \tag{3.1.57}$$

so that (3.1.55) becomes

$$\int_{\mathbb{R}} f(t)\, \mathrm{d}\lambda(t) = \sum_{\nu=1}^n \sum_{\sigma=0}^{2s} \lambda_\nu^{(\sigma)} f^{(\sigma)}(\tau_\nu) + R_{n,s}(f). \tag{3.1.58}$$

We then have necessarily $k \le n$, since otherwise $p = \omega_n$ would be admissible in (3.1.56), which would require $\int_{\mathbb{R}} \omega_n^{r+1}(t)\, \mathrm{d}\lambda(t) = 0$. This, when r is odd, is clearly impossible. The maximum degree of exactness of (3.1.58), therefore, is $d = (2s+2)n - 1$, and is achieved precisely if

$$\int_{\mathbb{R}} [\omega_n(t)]^{2s+1} p(t)\, \mathrm{d}\lambda(t) = 0 \quad \text{for all } p \in \mathbb{P}_{n-1}, \tag{3.1.59}$$

and the weights $\lambda_\nu^{(\sigma)}$ in (3.1.58) are determined by (Hermite) interpolation. This is the *Gauss–Turán quadrature formula*.

Recall from §1.2.4 that the (monic) polynomial ω_n satisfying (3.1.59) is the s-orthogonal polynomial $\omega_n = \pi_{n,s}$, which by Theorem 1.25 exists uniquely as the solution of the extremal problem

$$\min_{\pi \in \mathbb{P}_n^\circ} \int_{\mathbb{R}} [\pi(t)]^{2s+2}\, \mathrm{d}\lambda(t), \tag{3.1.60}$$

where $\mathbb{P}_n^\circ$ is the class of monic polynomials of degree n. Moreover, by Theorem 1.26, its zeros—the nodes τ_ν of (3.1.58)—are real, simple, and contained in the interior of the support interval of $\mathrm{d}\lambda$. The Gauss–Turán formula is thus seen to preserve many of the properties enjoyed by the ordinary Gauss quadrature rule. One of the important properties, the positivity of the weights, however, does not completely carry over. For the case $s = 1$, Turán already proved that $\lambda_\nu^{(2)} > 0$, while for general s, Micchelli (1972, Theorem 3) and Ossicini and Rosati (1978) prove $\lambda_\nu^{(\sigma)} > 0$ for even $\sigma \ge 0$. When σ is odd, $\lambda_\nu^{(\sigma)}$ may have either sign, in general.

Theorem 3.20 *If* $\mathrm{d}\lambda$ *is a symmetric measure* (cf. Definition 1.16) *and the nodes* τ_ν *are ordered* (either increasingly or decreasingly)*, then*

$$\left.\begin{aligned}\tau_{n+1-\nu}+\tau_\nu&=0\\ \lambda_{n+1-\nu}^{(\sigma)}&=(-1)^\sigma\lambda_\nu^{(\sigma)}\end{aligned}\right\}\ \nu=1,2,\dots,n. \tag{3.1.61}$$

In particular, $\lambda_{(n+1)/2}^{(\sigma)}=0$ *if* n *and* σ *are both odd.*

Proof The symmetry of the nodes follows from the fact that $\hat\pi_{n,s}(t)=(-1)^n\times\pi_{n,s}(-t)$ is a monic polynomial of degree n that satisfies the same power orthogonality condition as does $\pi_{n,s}$ and, hence, by uniqueness, must be identically equal to $\pi_{n,s}(t)$. The symmetry of the weights is a consequence of the symmetry of the underlying Hermite interpolation process. □

Example 3.21 Gauss–Turán formula for the Chebyshev measure $\mathrm{d}\lambda(t)=(1-t^2)^{-1/2}\,\mathrm{d}t$.

By a result of Bernstein (1930), the extremal polynomial of (3.1.60) is the monic Chebyshev polynomial $2^{1-n}T_n(t)$ for each $s\ge0$. Therefore, the Chebyshev points $\tau_\nu=\cos((2\nu-1)/2n)\pi$ serve as nodes for *all* Gauss–Turán formulae (3.1.58) with $s=0,1,2,\dots$, that is, there are weights $\lambda_\nu^{(\sigma)}$ such that

$$\int_{-1}^1 f(t)(1-t^2)^{-1/2}\,\mathrm{d}t=\sum_{\nu=1}^n\sum_{\sigma=0}^{2s}\lambda_\nu^{(\sigma)}f^{(\sigma)}(\tau_\nu)+R_{n,s}(f),\ \ s=0,1,2,\dots, \tag{3.1.62}$$

where $R_{n,s}(f)=0$ for all $f\in\mathbb{P}_{2(s+1)n-1}$. There are no simple explicit formulae for the weights $\lambda_\nu^{(\sigma)}$, but by a result of Kis (1957) they can be obtained, in principle, from the alternative trigonometric form of (3.1.62),

$$\int_{-1}^1 f(t)(1-t^2)^{-1/2}\,\mathrm{d}t=\frac{\pi}{ns!^2}\sum_{\nu=1}^n\sum_{j=0}^s\frac{S_j}{4^jn^{2j}}\,[D^{2j}f(\cos\theta)]_{\theta=\theta_\nu}+R_{n,s}(f), \tag{3.1.63}$$

where $D=\mathrm{d}/\mathrm{d}\theta$, $\theta_\nu=(2\nu-1)\pi/2n$, and S_{s-j}, $j=0,1,\dots,s$, are the elementary symmetric polynomials in the numbers $1^2,2^2,\dots,s^2$, that is,

$$S_s=1,\quad S_{s-1}=1^2+2^2+\cdots+s^2,\quad\dots\ ,\quad S_0=1^2\cdot2^2\cdots s^2.$$

For $s=1$, for example, one finds

$$\lambda_\nu^{(0)}=\frac{\pi}{n},\quad \lambda_\nu^{(1)}=-\frac{\tau_\nu}{4n^3},\quad \lambda_\nu^{(2)}=\frac{\pi}{4n^3}\,(1-\tau_\nu^2)\quad(s=1),$$

and for $s=2$,

$$\lambda_\nu^{(0)}=\frac{\pi}{n},\quad \lambda_\nu^{(1)}=-\frac{\pi\tau_\nu}{64n^5}\,(20n^2-1),\quad \lambda_\nu^{(2)}=\frac{\pi}{64n^5}\,[(20n^2-7)(1-\tau_\nu^2)+3],$$
$$\lambda_\nu^{(3)}=-\frac{3\pi\tau_\nu}{32n^5}\,(1-\tau_\nu^2),\quad \lambda_\nu^{(4)}=\frac{\pi}{64n^5}\,(1-\tau_\nu^2)^2\quad(s=2).$$

Formulae for $s = 3$ are given in Gautschi and Milovanović (1997, p. 215). Note that, indeed, $\lambda_\nu^{(\sigma)} > 0$ if σ is even.

3.1.3.2 *Computation of the Gauss–Turán formula* There are two separate issues: the generation of the s-orthogonal polynomials and their zeros τ_ν, and the computation of the weights $\lambda_\nu^{(\sigma)}$. We begin with the first.

The basic idea is to reinterpret the power orthogonality condition (3.1.59), where $\omega_n = \pi_{n,s}$, as an ordinary orthogonality condition relative to the (positive) measure $\mathrm{d}\lambda_{n,s}(t) = [\pi_{n,s}(t)]^{2s}\,\mathrm{d}\lambda(t)$,

$$\int_{\mathbb{R}} \pi_{n,s}(t) p(t)\,\mathrm{d}\lambda_{n,s}(t) = 0 \quad \text{for all } p \in \mathbb{P}_{n-1}. \tag{3.1.64}$$

This suggests to consider a sequence of $n+1$ (monic) polynomials $\pi_{0,s}, \pi_{1,s}, \dots,$ $\pi_{n,s}$ orthogonal with respect to the measure $\mathrm{d}\lambda_{n,s}$ and to generate them by the usual three-term recurrence relation. The last of these polynomials is the one we are actually interested in. The catch, of course, is that the measure depends on the (as yet unknown) polynomial $\pi_{n,s}$. Nevertheless, there must exist a three-term recurrence relation (1.3.2) for the polynomials $\pi_k = \pi_{k,s}$, with certain (unknown) coefficients α_k and β_k given by (1.3.3) and (1.3.4), where $\mathrm{d}\lambda$ is to be replaced by $\mathrm{d}\lambda_{n,s}$. Writing out the first n of formulae (1.3.3), and the first $n-1$ of (1.3.4), yields a system of $2n-1$ nonlinear equations

$$\boldsymbol{f}(\boldsymbol{\rho}) = \mathbf{0}, \quad \boldsymbol{\rho}^{\mathrm{T}} = [\alpha_0, \dots, \alpha_{n-1}; \beta_1 \dots, \beta_{n-1}], \tag{3.1.65}$$

where $\boldsymbol{f}^{\mathrm{T}} = [f_1, f_2, \dots, f_{2n-1}]$ is given by

$$\begin{aligned} f_{2\nu+1} &= \int_{\mathbb{R}} (\alpha_\nu - t)\pi_\nu^2(t)\pi_n^{2s}(t)\,\mathrm{d}\lambda(t), \quad \nu = 0, 1, \dots, n-1, \\ f_{2\nu} &= \int_{\mathbb{R}} (\beta_\nu \pi_{\nu-1}^2(t) - \pi_\nu^2(t))\pi_n^{2s}(t)\,\mathrm{d}\lambda(t), \quad \nu = 1, \dots, n-1. \end{aligned} \tag{3.1.66}$$

Each of the f_k is, indeed, a function of the coefficients $\alpha_0, \alpha_1, \dots; \beta_1, \beta_2 \dots,$ which appear on the right-hand sides of (3.1.66) either explicitly or implicitly through the polynomials $\pi_1, \pi_2, \dots, \pi_n$, which must be generated recursively by means of these coefficients. Thus, given a set of coefficients, the integrands in (3.1.66) can be computed recursively for any given t. Since they are polynomials of degrees $\le 2(s+1)n-1$, the integrals themselves can be computed exactly by an $(s+1)n$-point Gauss quadrature rule relative to the measure $\mathrm{d}\lambda$. The latter, in turn, can be computed as described in §3.1.1.1. The same quadrature rule can be used, if need be, to compute $\beta_0 = \int_{\mathbb{R}} [\pi_{n,s}(t)]^{2s}\,\mathrm{d}\lambda(t)$, once the coefficients α_ν and β_ν have been obtained.

In order to solve (3.1.65) by Newton's method, we need the Jacobian matrix $\partial \boldsymbol{f}/\partial \boldsymbol{\rho}$ of $\boldsymbol{f}$. This requires the auxiliary quantities

$$a_{\nu\mu} = \frac{\partial \pi_\nu}{\partial \alpha_\mu}, \ \mu = 0, 1, \dots, n-1; \ \ b_{\nu\mu} = \frac{\partial \pi_\nu}{\partial \beta_\mu}, \ \mu = 1, 2, \dots, n-1; \quad \nu = 0, 1, \dots, n,$$

which may be placed in two matrices $\boldsymbol{A}$ and $\boldsymbol{B}$ of dimensions $(n+1)\times n$ and $(n+1)\times(n-1)$, respectively. It is clear that $a_{\nu\mu}=b_{\nu\mu}=0$ if $\nu\le\mu$, so that $\boldsymbol{A}$ and $\boldsymbol{B}$ are lower triangular matrices with zeros on the diagonal. The μth column, $\mu=0,1,\dots,n-1$, of $\boldsymbol{A}$ is obtained by differentiating the three-term recurrence relation (1.3.2) with respect to α_μ. This yields the recursion

$$\begin{aligned} a_{\mu+1,\mu} &= -\pi_\mu(t), \quad a_{\mu\mu}=0,\\ a_{\nu+1,\mu} &= (t-\alpha_\nu)a_{\nu\mu}-\beta_\nu a_{\nu-1,\mu}, \quad \nu=\mu+1,\mu+2,\dots,n-1. \end{aligned}$$

Similarly, one finds for the μth column, $\mu=1,2,\dots,n-1$, of $\boldsymbol{B}$,

$$\begin{aligned} b_{\mu+1,\mu} &= -\pi_{\mu-1}(t), \quad b_{\mu\mu}=0,\\ b_{\nu+1,\mu} &= (t-\alpha_\nu)b_{\nu\mu}-\beta_\nu b_{\nu-1,\mu}, \quad \nu=\mu+1,\mu+2,\dots,n-1. \end{aligned}$$

Differentiating (3.1.66) with respect to α_μ and β_μ, we can express the elements of the Jacobian in terms of the auxiliary quantities $a_{\nu\mu}$ and $b_{\nu\mu}$ as follows:

$$\begin{aligned} \frac{\partial f_{2\nu+1}}{\partial\alpha_\mu} &= 2\int_{\mathbb{R}}\pi_n^{2s-1}(t)[(\alpha_\nu-t)p_{\nu\mu}(t)+\tfrac{1}{2}\delta_{\nu\mu}\pi_\nu^2(t)\pi_n(t)]\,\mathrm{d}\lambda(t),\\ \frac{\partial f_{2\nu+1}}{\partial\beta_\mu} &= 2\int_{\mathbb{R}}\pi_n^{2s-1}(t)(\alpha_\nu-t)q_{\nu\mu}(t)\,\mathrm{d}\lambda(t),\\ \frac{\partial f_{2\nu}}{\partial\alpha_\mu} &= 2\int_{\mathbb{R}}\pi_n^{2s-1}(t)(\beta_\nu p_{\nu-1,\mu}(t)-p_{\nu\mu}(t))\,\mathrm{d}\lambda(t),\\ \frac{\partial f_{2\nu}}{\partial\beta_\mu} &= 2\int_{\mathbb{R}}\pi_n^{2s-1}(t)[(\beta_\nu q_{\nu-1,\mu}(t)-q_{\nu\mu}(t))+\tfrac{1}{2}\delta_{\nu\mu}\pi_{\nu-1}^2(t)\pi_n(t)]\,\mathrm{d}\lambda(t)\ (\text{if } \nu>0), \end{aligned} \tag{3.1.67}$$

where

$$p_{\nu\mu}(t)=\pi_\nu(t)(a_{\nu\mu}\pi_n(t)+sa_{n\mu}\pi_\nu(t)), \quad q_{\nu\mu}(t)=\pi_\nu(t)(b_{\nu\mu}\pi_n(t)+sb_{n\mu}\pi_\nu(t)).$$

(When $\nu=0$ in the third relation of (3.1.67), one has $p_{-1,\mu}=0$ and $p_{0\mu}=sa_{n\mu}$.) By examining the degrees of the integrands in (3.1.67), one finds that the same $(s+1)n$-point Gauss quadrature rule applicable for (3.1.66) can also be applied to (3.1.67).

Newton's iteration for solving (3.1.65) can now easily be implemented. There remains the difficulty, however, of procuring good initial approximations to α_k, β_k, $k=0,1,\dots,n-1$. For given n and s, a natural choice are the coefficients $\alpha_k(\mathrm{d}\lambda)$ and $\beta_k(\mathrm{d}\lambda)$ corresponding to $s=0$, which are assumed known. If this does not work, we recommend one of two alternatives, or a combination of both: (1) Lower the accuracy requirement until convergence is achieved, and then use the results as new initial approximations for a next higher accuracy level. Continue in this manner until the desired accuracy level is attained. (2) Use a discrete

homotopy approach in the variable s by considering a chain of problems corresponding to values $s' = 0, 1, \ldots, s$ of s. The first problem in this chain has the solution $\alpha_k(\mathrm{d}\lambda)$ and $\beta_k(\mathrm{d}\lambda)$, and the last problem is the one we want to solve. Each problem, starting with $s' = 1$, is now solved in succession, using as intitial approximations the solution of the preceding problem. Once Newton's method has converged, the solution vector $\boldsymbol{\rho}$ of the recursion coefficients α_k and β_k yields the Jacobi matrix $\boldsymbol{J}_n(\mathrm{d}\lambda_{n,s})$, whose eigenvalues are the desired nodes τ_ν.

As far as the weights are concerned, it turns out that for each ν the weights $\lambda_\nu^{(0)}, \lambda_\nu^{(1)}, \ldots, \lambda_\nu^{(2s)}$ are the solution of a triangular system of linear equations (for details, see Gautschi and Milovanović (1997, §3)). Indeed, let[4]

$$\hat{\lambda}_\sigma = \sigma! \lambda_\nu^{(\sigma)}, \quad \sigma = 0, 1, \ldots, 2s,$$

and

$$\hat{\mu}_\sigma = \int_{\mathbb{R}} (t - \tau_\nu)^\sigma \left(\prod_{\substack{\mu=1 \\ \mu \neq \nu}}^{n} \frac{t - \tau_\mu}{\tau_\nu - \tau_\mu} \right)^{2s+1} \mathrm{d}\lambda(t), \quad \sigma = 0, 1, \ldots, 2s,$$

and let $\hat{\boldsymbol{\lambda}}$, $\hat{\boldsymbol{\mu}}$ be the respective vectors of dimension $2s + 1$. Define the upper triangular Toeplitz matrix $\hat{\boldsymbol{A}} = [\hat{a}_{ik}]$ of order $2s + 1$ with diagonal elements

$$\hat{a}_{kk} = 1, \quad k = 1, 2, \ldots, 2s + 1,$$

and the jth upper paradiagonal, $j = 1, 2, \ldots, 2s$, defined by

$$\hat{a}_{k,k+j} = -\frac{2s+1}{j} \sum_{\ell=1}^{j} u_\ell \hat{a}_{\ell j}, \quad k = 1, 2, \ldots, 2s + 1 - j,$$

where

$$u_\ell = \sum_{\substack{\mu=1 \\ \mu \neq \nu}}^{n} \left(\frac{1}{\tau_\mu - \tau_\nu} \right)^\ell, \quad \ell = 1, 2, \ldots, 2s.$$

Then,

$$\hat{\boldsymbol{A}} \hat{\boldsymbol{\lambda}} = \hat{\boldsymbol{\mu}}. \tag{3.1.68}$$

Since the integral defining $\hat{\mu}_\sigma$ involves a polynomial of degree at most $2(s+1)n - n - 1$, it can be computed exactly by the same $(s+1)n$-point Gauss formula used before in (3.1.66) and (3.1.67).

The procedure is implemented in the `OPQ` routine `turan.m`.

Example 3.22 Symmetric measure and $n = 2$, $s = 1$ or $s = 2$.

[4] In the corresponding formula for b_k on p. 213 of Gautschi and Milovanović (1997), the factorial sign was inadvertently omitted.

From the proof of Theorem 3.20, it follows that $\alpha_k = 0$ for all k, and hence $\pi_1(t) = t$, $\pi_2(t) = t\pi_1(t) - \beta_1 = t^2 - \beta_1$, so that the system of equations (3.1.65), for $n = 2$, can be written as

$$\begin{aligned}
&\int_{\mathbb{R}} t(t^2 - \beta_1)^{2s}\, \mathrm{d}\lambda(t) = 0,\\
&\int_{\mathbb{R}} t^3(t^2 - \beta_1)^{2s}\, \mathrm{d}\lambda(t) = 0,\\
&\int_{\mathbb{R}} (t^2 - \beta_1)^{2s+1}\, \mathrm{d}\lambda(t) = 0.
\end{aligned}$$

The first two equations are automatically satisfied by symmetry. The third equation, for $s = 1$, is a cubic equation in β_1,

$$\mu_0\beta_1^3 - 3\mu_2\beta_1^2 + 3\mu_4\beta_1 - \mu_6 = 0 \quad (s = 1),$$

where μ_k are the moments of $\mathrm{d}\lambda$. By the uniqueness of π_2, there can be only *one* real (in fact, positive) root. Likewise, for $s = 2$, one obtains for β_1 a quintic equation,

$$\mu_0\beta_1^5 - 5\mu_2\beta_1^4 + 10\mu_4\beta_1^3 - 10\mu_6\beta_1^2 + 5\mu_8\beta_1 - \mu_{10} = 0 \quad (s = 2).$$

By straightforward, though tedious, calculations, the generating elements for the Toeplitz matrix $\hat{\boldsymbol{A}}$ for $\nu = 1$ and $\nu = 2$ are found to be (assuming $\tau_1 > 0 > \tau_2 = -\tau_1$)

$$\hat{a}_{11} = 1,\ \hat{a}_{12} = -\tfrac{3}{2}(-1)^\nu\tau_1^{-1},\ \hat{a}_{13} = \tfrac{3}{4}\,\tau_1^{-2} \quad (s = 1),$$

and

$$\hat{a}_{11} = 1,\ \hat{a}_{12} = -\tfrac{5}{2}(-1)^\nu\tau_1^{-1},\ \hat{a}_{13} = \tfrac{5}{2}\tau_1^{-2},\ \hat{a}_{14} = -\tfrac{5}{4}(-1)^\nu\tau_1^{-3},\ \hat{a}_{15} = \tfrac{5}{16}\tau_1^{-4} \quad (s = 2),$$

while the components of the vectors $\hat{\boldsymbol{\mu}}$ are, for $s = 1$,

$$\begin{aligned}
\hat{\mu}_0 &= \tfrac{1}{8}(\mu_0 - 3(-1)^\nu\mu_1\tau_1^{-1} + 3\mu_2\tau_1^{-2} - (-1)^\nu\mu_3\tau_1^{-3}),\\
\hat{\mu}_1 &= \tfrac{1}{8}((-1)^\nu\mu_0\tau_1 - 2\mu_1 + 2\mu_3\tau_1^{-2} - (-1)^\nu\mu_4\tau_1^{-3}),\\
\hat{\mu}_2 &= \tfrac{1}{8}(\mu_0\tau_1^2 - (-1)^\nu\mu_1\tau_1 - 2\mu_2 + 2(-1)^\nu\mu_3\tau_1^{-1} + \mu_4\tau_1^{-2} - (-1)^\nu\mu_5\tau_1^{-3}),
\end{aligned}$$

and, for $s = 2$,

$$\hat{\mu}_0 = \tfrac{1}{32}(\mu_0 - 5(-1)^\nu\mu_1\tau_1^{-1} + 10\mu_2\tau_1^{-2} - 10(-1)^\nu\mu_3\tau_1^{-3} + 5\mu_4\tau_1^{-4} - (-1)^\nu\mu_5\tau_1^{-5}),$$
$$\hat{\mu}_1 = \tfrac{1}{32}((-1)^\nu\mu_0\tau_1 - 4\mu_1 + 5(-1)^\nu\mu_2\tau_1^{-1} - 5(-1)^\nu\mu_4\tau_1^{-3} + 4\mu_5\tau_1^{-4} - (-1)^\nu\mu_6\tau_1^{-5}),$$
$$\hat{\mu}_2 = \tfrac{1}{32}(\mu_0\tau_1^2 - 3(-1)^\nu\mu_1\tau_1 + \mu_2 + 5(-1)^\nu\mu_3\tau_1^{-1} - 5\mu_4\tau_1^{-2} - (-1)^\nu\mu_5\tau_1^{-3}$$
$$+3\mu_6\tau_1^{-4} - (-1)^\nu\mu_7\tau_1^{-5}),$$
$$\hat{\mu}_3 = \tfrac{1}{32}((-1)^\nu\mu_0\tau_1^3 - 2\mu_1\tau_1^2 - 2(-1)^\nu\mu_2\tau_1 + 6\mu_3 - 6\mu_5\tau_1^{-2} + 2(-1)^\nu\mu_6\tau_1^{-3}$$
$$+2\mu_7\tau_1^{-4} - (-1)^\nu\mu_8\tau_1^{-5}),$$
$$\hat{\mu}_4 = \tfrac{1}{32}(\mu_0\tau_1^4 - (-1)^\nu\mu_1\tau_1^3 - 4\mu_2\tau_1^2 + 4(-1)^\nu\mu_3\tau_1 + 6\mu_4 - 6(-1)^\nu\mu_5\tau_1^{-1} - 4\mu_6\tau_1^{-2}$$
$$+4(-1)^\nu\mu_7\tau_1^{-3} + \mu_8\tau_1^{-4} - (-1)^\nu\mu_9\tau_1^{-5}).$$

The explicit formulae assembled here have been found useful in the development and testing of the routine `turan.m`.

Example 3.23 Gauss–Turán formulae for the Legendre measure.

Here, $\mathrm{d}\lambda(t) = \mathrm{d}t$ on $[-1, 1]$. The Matlab script

```
eps0=1.e-14;
ab0=r_jacobi(21); hom=1;
for n=2:7
   for s=1:2
     xw=turan(n,s,eps0,ab0,hom);
   end
end
```

computes formulae (3.1.58) for $n = 2, 3, \ldots, 7$, $s = 1$, and $s = 2$, with a requested accuracy level of 10^{-14}. The value `hom`=1 of the parameter `hom` means that homotopy in the variable s is used. Newton's method in this case never required more than seven iterations. Without homotopy (`hom`=0), it required as much as 12 iterations (for $n = 7$ and $s = 2$). Comparing the results with the 20-decimal values in Tables 1 and 2 of Stroud and Stancu (1965), we found that the error is usually a few units in the 16th decimal place, more precisely, 1–2 units for the weights $\lambda_\nu^{(\sigma)}$, $1 \le \sigma \le 2s$, up to 18 units for $\lambda_\nu^{(0)}$, and less than 6 units for the nodes; see the `OPQ` routine `Example3_23.m`. This high degree of accuracy is achieved in spite of the fact that the condition of the Jacobian matrices in Newton's method, and especially that of the matrices $\hat{\boldsymbol{A}}$, becomes fairly bad with increasing n. For $n = 7$ and $s = 2$, the respective condition numbers are 2.0×10^4 and as large as 5.3×10^{10}.

Example 3.24 Gauss–Turán formulae for the Laguerre and Hermite measures.

Similarly as in Example 3.23, and with comparable success, we reproduced the results for the Laguerre measure given in Table 5 of Stroud and Stancu (1965). It was observed, however, that the Jacobian matrices become ill conditioned much more rapidly, reaching a condition number of the order 10^9 already for $n = 4$, when $s = 2$. The method failed to converge when $n = 5$. For the Hermite measure, we reproduced all results in Tables 3 and 4 of Stroud and Stancu (1965) except

those for $n = 7$. However, $n = 6$ and $s = 1$ required 26 iterations for Newton's method to converge. It failed to converge when $n = 7$, in part because of the ill-conditioning of the Jacobian matrices. See the `OPQ` routine `Example3_24.m`.

3.1.4 *Quadrature formulae based on rational functions*

The Gauss and Gauss-type quadrature formulae discussed so far, including the Gauss–Kronrod and Gauss–Turán formulae, are all polynomial-based; they are optimal with respect to polynomial degree of exactness. This is meaningful if the functions to be integrated are indeed polynomial-like, but may be questionable otherwise. As is often the case, for example, the integrand has poles outside the interval of integration, perhaps even infinitely many. It would then be natural to require exactness not only for polynomials of certain degrees, but also for elementary rational functions having the same poles, or at least the more important ones among them (those closest to the interval of integration). This calls for quadrature rules of mixed polynomial/rational degree of exactness. The present section is devoted to a study of these "rational" quadrature rules.

3.1.4.1 *Rational Gauss formulae* We begin with a quadrature rule of the usual form

$$\int_{\mathbb{R}} f(t)\,\mathrm{d}\lambda(t) = \sum_{\nu=1}^{n} \lambda_\nu f(\tau_\nu) + R_n(f), \tag{3.1.69}$$

where $\mathrm{d}\lambda$ is a positive measure and f is assumed to have poles in the complex plane away from the support interval of $\mathrm{d}\lambda$. Let m be an integer satisfying

$$0 \le m \le 2n \tag{3.1.70}$$

and $\mathbb{Q}_m$ the linear space of rational functions defined by

$$\mathbb{Q}_m = \mathrm{span}\{r:\ r(t) = (1+\zeta_\mu t)^{-s},\ s = 1, 2, \ldots, s_\mu;\ \mu = 1, 2, \ldots, M\},$$
$$\sum_{\mu=1}^{M} s_\mu = m. \tag{3.1.71}$$

Thus, $\mathbb{Q}_m$ is a space of dimension m consisting of all linear combinations of the elementary rational functions $(1+\zeta_\mu t)^{-s}$. The parameters ζ_μ are distinct real or complex numbers meant to be chosen such that $-1/\zeta_\mu$, the poles of the elementary rational functions, are equal to, or approximate, the most relevant poles of f. The integers s_μ are the multiplicities of the respective poles. We assume that

$$\zeta_\mu \ne 0, \quad 1 + t\zeta_\mu \ne 0 \ \text{ for } t \in [a, b], \quad \mu = 1, 2, \ldots, M, \tag{3.1.72}$$

where $[a, b]$ is the support interval of $\mathrm{d}\lambda$. We denote by $\mathbb{S}_{2n}$ the space of dimension $2n$ made up of the space $\mathbb{Q}_m$ of dimension m adjoined by the space of polynomials of degree $\le 2n - 1 - m$,

$$\mathbb{S}_{2n} = \mathbb{Q}_m \oplus \mathbb{P}_{2n-1-m}. \tag{3.1.73}$$

Our objective is to construct formula (3.1.69) in such a way that

$$R_n(f) = 0 \quad \text{for all } f \in \mathbb{S}_{2n}. \tag{3.1.74}$$

The integer m is a parameter that can be chosen at our discretion, subject to (3.1.70). In the limit case $m = 0$, the space $\mathbb{Q}_m$ is empty, $\mathbb{S}_{2n} = \mathbb{P}_{2n-1}$, and we are back in the polynomial case. The other extreme, $m = 2n$, yields for $\mathbb{S}_{2n}$ a space of genuinely rational functions ($\mathbb{P}_{-1}$ is empty), and the resulting quadrature formula will not be exact for any polynomial, not even constants. In practice, a middle ground is probably best, that is, a value of m about halfway between 0 and $2n$.

The manner in which the desired quadrature rule can be constructed is the content of the following theorem.

Theorem 3.25 *Define the polynomial* (of exact degree m)

$$\omega_m(t) = \prod_{\mu=1}^{M} (1 + \zeta_\mu t)^{s_\mu}. \tag{3.1.75}$$

Assume that the measure $\mathrm{d}\lambda/\omega_m$ *admits an* n*-point* (polynomial) *Gaussian quadrature formula*

$$\int_{\mathbb{R}} p(t) \frac{\mathrm{d}\lambda(t)}{\omega_m(t)} = \sum_{\nu=1}^{n} \lambda_\nu^G p(\tau_\nu^G) \quad \textit{for all } p \in \mathbb{P}_{2n-1}, \tag{3.1.76}$$

having distinct nodes τ_ν^G *contained in the support interval* $[a, b]$ *of* $\mathrm{d}\lambda$*. Then,*

$$\tau_\nu = \tau_\nu^G, \quad \lambda_\nu = \lambda_\nu^G \omega_m(\tau_\nu^G), \quad \nu = 1, 2, \ldots, n, \tag{3.1.77}$$

yields the desired formula (3.1.69) satisfying (3.1.74).

Conversely, if (3.1.69) and (3.1.74) hold with τ_ν *in the support interval of* $\mathrm{d}\lambda$*, then so does (3.1.76) with* τ_ν^G *and* λ_ν^G *as obtained from (3.1.77).*

Proof Assume first (3.1.76), with all τ_ν^G contained in the support interval of $\mathrm{d}\lambda$. Let

$$q_{\mu,s}(t) = \frac{\omega_m(t)}{(1 + \zeta_\mu t)^s}, \quad \mu = 1, 2, \ldots, M; \ s = 1, 2, \ldots, s_\mu. \tag{3.1.78}$$

Since $m \le 2n$ and $s \ge 1$, one has $q_{\mu,s} \in \mathbb{P}_{m-s} \subseteq \mathbb{P}_{2n-1}$, and, therefore, by (3.1.76),

$$\begin{aligned} \int_{\mathbb{R}} \frac{\mathrm{d}\lambda(t)}{(1 + \zeta_\mu t)^s} &= \int_{\mathbb{R}} q_{\mu,s}(t) \frac{\mathrm{d}\lambda(t)}{\omega_m(t)} = \sum_{\nu=1}^{n} \lambda_\nu^G q_{\mu,s}(\tau_\nu^G) \\ &= \sum_{\nu=1}^{n} \lambda_\nu^G \frac{\omega_m(\tau_\nu^G)}{(1 + \zeta_\mu \tau_\nu^G)^s} = \sum_{\nu=1}^{n} \frac{\lambda_\nu}{(1 + \zeta_\mu \tau_\nu)^s}. \end{aligned}$$

Here, (3.1.77) has been used in the last step, and none of the denominators on the far right vanishes because of (3.1.72) and the assumption $\tau_\nu \in [a, b]$. This proves

(3.1.74) for the rational part $\mathbb{Q}_m$ of $\mathbb{S}_{2n}$. The assertion for the polynomial part $\mathbb{P}_{2n-1-m}$ follows similarly: If p is any polynomial in $\mathbb{P}_{2n-1-m}$, then $p\omega_m \in \mathbb{P}_{2n-1}$, and (3.1.76) yields

$$\int_{\mathbb{R}} p(t)\,\mathrm{d}\lambda(t) = \int_{\mathbb{R}} p(t)\omega_m(t)\frac{\mathrm{d}\lambda(t)}{\omega_m(t)} = \sum_{\nu=1}^{n} \lambda_\nu^G p(\tau_\nu^G)\omega_m(\tau_\nu^G) = \sum_{\nu=1}^{n} \lambda_\nu p(\tau_\nu),$$

again by (3.1.77).

To prove the converse, note first of all that λ_ν^G is well defined by (3.1.77), since $\omega_m(\tau_\nu^G) \neq 0$ by (3.1.72) and the assumption $\tau_\nu^G \in [a,b]$. One then verifies that (3.1.76) holds for all polynomials (3.1.78) (of degrees $<m$) and all polynomials of the form $p\omega_m$, $p \in \mathbb{P}_{2n-1-m}$, the union of which spans $\mathbb{P}_{2n-1}$. □

Remark to Theorem 3.25 It is sometimes useful to consider in place of (3.1.69) the more specific quadrature rule

$$\int_{\mathbb{R}} f(t)s(t)\,\mathrm{d}\lambda(t) = \sum_{\nu=1}^{n} \lambda_\nu f(\tau_\nu) + R_n(f), \tag{3.1.79}$$

where s is a function that exhibits difficult behavior unrelated to the poles of f, and $\mathrm{d}\lambda$ is one of the standard integration measures. Theorem 3.25 then remains valid if (3.1.76) is replaced by

$$\int_{\mathbb{R}} p(t)\frac{s(t)\,\mathrm{d}\lambda(t)}{\omega_m(t)} = \sum_{\nu=1}^{n} \lambda_\nu^G p(\tau_\nu^G), \quad p \in \mathbb{P}_{2n-1}. \tag{3.1.80}$$

Since the numbers ζ_μ, in general, are complex, the "modified measure" $\mathrm{d}\lambda/\omega_m$ in (3.1.76) may be complex-valued, and the existence of the Gauss formula (3.1.76) is not ensured. There is no such uncertainty, however, if ω_m is of constant sign on $[a,b]$, a situation that occurs in a number of special cases, all of interest in applications. We mention here some of the more important ones.

Example 3.26 Simple real poles.

Here, all $s_\mu = 1$ (hence $M = m$), and $\zeta_\mu = \xi_\mu$ are real and distinct, with $\xi_\mu \neq 0$, $\mu = 1, 2, \ldots, m$. The polynomial ω_m then becomes

$$\omega_m(t) = \prod_{\mu=1}^{m} (1 + \xi_\mu t).$$

Since by assumption ω_m does not vanish on the support interval $[a,b]$, the polynomial ω_m has constant sign on $[a,b]$, that is, $\mathrm{d}\lambda/\omega_m$ is a (positive or negative) definite measure. All of its moments evidently exist. The Gauss formula (3.1.76), therefore, exists uniquely for every n, and all its nodes are in $[a,b]$.

Example 3.27 Simple conjugate complex poles.

This is the case where all $s_\mu = 1$, m is even, and

$$\zeta_\mu = \xi_\nu + \mathrm{i}\eta_\nu, \quad \zeta_{\mu+1} = \xi_\nu - \mathrm{i}\eta_\nu \quad (\nu = 1 + \lfloor \mu/2 \rfloor),$$
$$\mu(\text{odd}) = 1, 3, \ldots, m-1,$$

where all ξ_ν are real and all η_ν positive. Then,

$$\omega_m(t) = \prod_{\nu=1}^{m/2} [(1+\xi_\nu t)^2 + \eta_\nu^2 t^2], \quad 2 \le m(\text{even}) \le 2n.$$

This is clearly positive on $\mathbb{R}$, and the hypotheses of Theorem 3.25 are satisfied.

Example 3.28 Same as Examples 3.26 or 3.27, but with $s_\mu = 2$ (hence $m = 2M$).

Example 3.29 Simple conjugate complex poles plus a real simple pole.

Here, all $s_\mu = 1$, m is odd ≥ 3, and

$$\zeta_\mu = \xi_\nu + \mathrm{i}\eta_\nu, \quad \zeta_{\mu+1} = \xi_\nu - \mathrm{i}\eta_\nu \quad (\nu = 1 + \lfloor \mu/2 \rfloor),$$
$$\mu(\text{odd}) = 1, 3, \ldots, m-2,$$
$$\zeta_m = \xi_m \in \mathbb{R},$$

with $\xi_\nu \in \mathbb{R}$, $\eta_\nu > 0$. This yields

$$\omega_m(t) = (1+\xi_m t) \prod_{\nu=1}^{(m-1)/2} [(1+\xi_\nu t)^2 + \eta_\nu^2 t^2],$$

which again has constant sign on $[a, b]$.

Example 3.30 Same as Example 3.29, but with two simple poles instead of one.

Note that all weights λ_ν in (3.1.69) are positive in each of these examples. This is clear if $\omega_m > 0$ on $[a, b]$, but also if $\omega_m < 0$, since then $\lambda_\nu^G < 0$ in (3.1.76) and thus $\lambda_\nu > 0$ by (3.1.77).

Given an ω_m of constant sign on $[a, b]$, the problem thus boils down to construct the Gauss quadrature rule (3.1.76) for the measure $\mathrm{d}\hat{\lambda}_m = \mathrm{d}\lambda/\omega_m$ or, what suffices in view of §3.1.1, the computation of the first $2n$ recurrence coefficients $\hat{\alpha}_k = \alpha_k(\mathrm{d}\hat{\lambda}_m)$, $\hat{\beta}_k = \beta_k(\mathrm{d}\hat{\lambda}_m)$, $k = 0, 1, \ldots, n-1$. Unless some of the zeros of ω_m, that is, some of the respective poles, are close to the interval $[a, b]$, a simple-minded discretization method (cf. §2.2.4) will do, the discretizations being accomplished by Gaussian quadrature rules relative to the measure $\mathrm{d}\lambda$. This is implemented in the `OPQ` routine `r_mod.m`, which calls on the routine `mcdis.m` to do the discretization. The output $\hat{\alpha}_k$, $\hat{\beta}_k$, $k = 0, 1, \ldots, n-1$, of the routine

`r_mod.m` is then fed into the routine `gauss_rational.m`, which generates the desired n-point rational Gauss formula according to Theorem 3.25. In the case of "difficult" poles, that is, poles close to $[a, b]$, additional work is required, which will be described in §3.1.4.2.

Example 3.31 The integral $\int_{-1}^{1} (\pi t/\omega)/\sin(\pi t/\omega)\,\mathrm{d}t$, $\omega > 1$.

The poles of the integrand are all simple and located at the integer multiples of ω; we are in the case of Example 3.26. To set up the space $\mathbb{Q}_m$, it is natural to let m be even and to incorporate the m poles closest to, and on either side of, the interval $[-1, 1]$. The corresponding values of ξ_ν (the negative reciprocals of the poles) are then

$$\xi_\nu = \frac{(-1)^\nu}{\lfloor (\nu+1)/2 \rfloor \omega}, \quad \nu = 1, 2, \ldots, m. \tag{3.1.81}$$

The discretization procedure described for computing the quadrature rule (3.1.76) works quite well, unless ω is very close to 1. For this latter case, see Example 3.34. Typical choices of m are $m = 2n$, $m = 2\lfloor (n+1)/2 \rfloor$, and $m = 2$. For these, and also for $m = 0$, selected results produced by the rational Gauss quadrature rule are shown for $\omega = 1.1$ in Table 3.1; they are obtained by the `OPQ` routine `Example3_31.m`, the core of which looks as follows:

Table 3.1 *The integral of Example 3.31 with* $\omega = 1.1$ *evaluated by rational Gauss quadrature.*

n	m	Integral	Error	`Ncap`	`kount`
1	2	3.34897468149577	2.504(–01)	51	16
4	8	4.46777134878307	5.143(–07)	49	8
7	14	4.46777364638772	9.741(–15)	57	6
10	20	4.46777364638777	0.000(+00)	81	6
1	2	3.34897468149577	2.504(–01)	51	16
4	4	4.46773974921780	7.587(–06)	49	8
7	8	4.46777364638446	7.399(–13)	57	6
10	10	4.46777364638776	1.392(–15)	81	6
1	2	3.34897468149577	2.504(–01)	51	16
4	2	4.46735807863000	9.302(–05)	49	8
7	2	4.46777355977115	1.939(–08)	57	6
10	2	4.46777364637083	3.792(–12)	81	6
1	0	2.00000000000000	5.524(–01)	—	—
4	0	4.24804106331922	4.918(–02)	—	—
7	0	4.45139788821468	3.665(–03)	—	—
10	0	4.46659960850924	2.628(–04)	—	—

```
ab0=r_jacobi(Nmax);
eps0=100*eps; sgn=1;
for m=1:M
   sgn=-sgn;
   Z(m,1)=sgn/(om*floor((m+1)/2)); Z(m,2)=1;
end
[abmod,Ncap,kount]=r_mod(N,ab0);
xw=gauss_rational(N,abmod);
```

The first command provides sufficiently many (`Nmax`) recursion coefficients for the Legendre measure $\mathrm{d}\lambda(t) = \mathrm{d}t$ on $[-1, 1]$. The choice `Nmax` =100 turned out to be adequate in all cases. The error tolerance `eps0` is used in the routine `mcdis.m` (called by `r_mod.m`), which also returns the integers `Ncap` and `kount`. They indicate the maximum number of Legendre recurrence coefficients, resp. the number of iterations, actually needed for the discretization process to converge. The array `Z` containing the ζ_μ and their multiplicities is used in the quadrature routine that generates the discretizations in `mcdis.m`. The (relative) errors shown in Table 3.1 were determined by comparison with results obtained by Maple to 20 decimals. It can be seen that incorporating the maximum number $m = 2n$ of poles yields the best results in this example. The accuracy deteriorates noticeably as m is decreased and is distinctly inferior when $m = 0$ (ordinary Gauss–Legendre quadrature).

Example 3.32 The integral $\int_0^1 \Gamma(1+t)t^{-1/2}\,\mathrm{d}t/(t+\omega)$, $\omega > 0$.

The measure here is $\mathrm{d}\lambda(t) = t^{-1/2}\,\mathrm{d}t$ on $[0, 1]$, and the poles are at $-\omega$ and at the negative natural numbers. Accordingly, we take

$$\xi_\nu = \frac{1}{\nu}\,, \quad \nu = 1, 2, \ldots, m-1; \quad \xi_m = \frac{1}{\omega}\,.$$

Selected results for $\omega = 0.1$, $m = 2n$, $m = n$, $m = 2$, and $m = 0$, analogous to those in Example 3.31, are produced by the `OPQ` routine `Example3_32.m` and are shown in Table 3.2. The core of the routine is almost identical to the one exhibited in Example 3.31, except for the obvious change in the generation of ξ_ν and the fact that we now need the routine `r_jacobi01(Nmax,0,-1/2)`. In this example, the results for $m = n$, and even those for $m = 2$, are slightly more accurate than those for $m = 2n$ (except when $n = m = 1$). The strong showing of $m = 2$ in this example, compared to Example 3.31, may at first surprise, but on reflection seems quite natural, given that the two most relevant poles in Example 3.31 are at the same distance from the support interval, whereas here they are not.

3.1.4.2 *Difficult poles* Poles that lie close to the support interval $[a, b]$ of $\mathrm{d}\lambda$ are difficult to handle by the discretization procedure in `mcdis.m`, since the measure $\mathrm{d}\hat{\lambda}_m = \mathrm{d}\lambda/\omega_m$ is nearly singular. It is better, in such cases, to first process the "benign" poles, that is, apply the procedure described in §3.1.4.1 to the measure $\mathrm{d}\tilde{\lambda} = \mathrm{d}\lambda/\tilde{\omega}_m$, where $\tilde{\omega}_m$ is the (constant-sign) polynomial corresponding

Table 3.2 *The integral of Example 3.32 with* $\omega = 0.1$ *evaluated by rational Gauss quadrature.*

n	m	Integral	Error	`Ncap`	`kount`
1	2	7.54645695430477	1.642(–02)	31	13
4	8	7.67246131529514	1.657(–07)	41	7
7	14	7.67246258637016	5.163(–14)	57	6
10	20	7.67246258637055	1.158(–15)	61	5
1	1	7.46180867023317	2.746(–02)	31	13
4	4	7.67246240210902	2.402(–08)	41	7
7	7	7.67246258637054	2.894(–15)	57	6
10	10	7.67246258637056	5.788(–16)	61	5
1	2	7.54645695430477	1.642(–02)	31	13
4	2	7.67246253098169	7.219(–09)	41	7
7	2	7.67246258637053	3.936(–15)	57	6
10	2	7.67246258637055	1.042(–15)	61	5
1	0	4.12144389955038	4.628(–01)	—	—
4	0	7.56688893903608	1.376(–02)	—	—
7	0	7.66991858256827	3.316(–04)	—	—
10	0	7.67240170362946	7.935(–06)	—	—

to all poles other than the difficult ones, and then do some postprocessing to incorporate the difficult poles. We describe the relevant procedures in the special (but important) case where all benign poles are simple and either all real, or all complex occurring in conjugate complex pairs. With regard to the difficult poles, we assume that there is either one such pole, which is real and simple, or a pair of simple real poles located symmetrically with respect to the origin.

We begin with the case of a single difficult pole $x \in \mathbb{R}$. Suppose we have already generated by the method of §3.1.4.1 sufficiently many recursion coefficients $\tilde{\alpha}_k$ and $\tilde{\beta}_k$ for the (partially modified) measure $\mathrm{d}\tilde{\lambda} = \mathrm{d}\lambda/\tilde{\omega}_m$. The problem then is to compute the recursion coefficients $\hat{\alpha}_k$ and $\hat{\beta}_k$ for the (fully modified) measure

$$\mathrm{d}\hat{\lambda}(t) = \frac{\mathrm{d}\tilde{\lambda}(t)}{t - x}\,, \tag{3.1.82}$$

where x is close to, but outside the support interval $[a, b]$ of $\mathrm{d}\tilde{\lambda}$ (or of $\mathrm{d}\lambda$, which is the same). This is precisely the problem discussed in §2.4.4 and can be solved by Algorithm 2.8. Recall, however, that this algorithm requires knowledge of the Cauchy integral

$$\rho_0(x; \mathrm{d}\tilde{\lambda}) = \int_{\mathbb{R}} \frac{\mathrm{d}\tilde{\lambda}(t)}{x - t}\,. \tag{3.1.83}$$

One possibility of computing it is to apply the continued fraction algorithm of §2.3.2. Unfortunately, and especially when x is close to $[a,b]$, as we assume here, this would require a large number of recurrence coefficients $\tilde{\alpha}_k$ and $\tilde{\beta}_k$. We prefer another technique that relies more on the original measure $\mathrm{d}\lambda$. It is based on the decomposition of $\tilde{\omega}_m^{-1}$ into partial fractions. We consider separately the case where all zeros of $\tilde{\omega}_m$ are real, and the case where all are complex, occurring in conjugate complex pairs.

In the first case,

$$\frac{1}{\tilde{\omega}_m(t)} = \frac{1}{\prod_\nu (1+\xi_\nu t)} = \sum_\nu \frac{c_\nu/\xi_\nu}{1/\xi_\nu + t}\,,$$

where the sum and product are extended over all benign poles (or, perhaps, approximations thereof), and where

$$c_\nu = \prod_{\mu\neq\nu} \frac{1}{1-\xi_\mu/\xi_\nu}\,. \tag{3.1.84}$$

Empty products (if there is only one, or no, benign pole) are understood to be equal to 1. We then have from (3.1.83), since $\mathrm{d}\tilde{\lambda} = \mathrm{d}\lambda/\tilde{\omega}_m$,

$$\rho_0(x;\mathrm{d}\tilde{\lambda}) = \int_{\mathbb{R}} \frac{\mathrm{d}\lambda(t)}{(x-t)\tilde{\omega}_m(t)} = \sum_\nu \int_{\mathbb{R}} \frac{1}{x-t}\,\frac{c_\nu/\xi_\nu}{1/\xi_\nu+t}\,\mathrm{d}\lambda(t).$$

Writing

$$\frac{1}{x-t}\,\frac{1}{1/\xi_\nu+t} = \frac{\xi_\nu}{1+\xi_\nu x}\left(\frac{1}{x-t}+\frac{1}{1/\xi_\nu+t}\right),$$

we get

$$\rho_0(x;\mathrm{d}\tilde{\lambda}) = \sum_\nu \frac{c_\nu}{1+\xi_\nu x}\,[\rho_0(x;\mathrm{d}\lambda) - \rho_0(-1/\xi_\nu;\mathrm{d}\lambda)]. \tag{3.1.85}$$

Both terms in brackets can be computed by the continued fraction algorithm alluded to above, but now for the underlying measure $\mathrm{d}\lambda$, which is usually one of the classical measures. The required recursion coefficients $\alpha_k = \alpha_k(\mathrm{d}\lambda)$ and $\beta_k = \beta_k(\mathrm{d}\lambda)$, therefore, are easily generated, in large numbers if necessary. For special measures, the Cauchy integral $\rho_0(x;\mathrm{d}\lambda)$ is known explicitly (cf. Examples 3.33 and 3.34); for others (cf. Example 3.36), it may be evaluated analytically.

In the second case of conjugate complex zeros, similar ideas apply, but they are a bit more complicated. The partial fraction decomposition of $\tilde{\omega}_m^{-1}$ now has the form

$$\frac{1}{\tilde{\omega}_m(t)} = \sum_\nu \frac{c_\nu + d_\nu t}{(t+1/\zeta_\nu)(t+1/\overline{\zeta}_\nu)}\,, \tag{3.1.86}$$

where the sum is extended over all pairs of conjugate complex (benign) poles. By an elementary computation one finds

$$c_\nu = \frac{\mathrm{Im}(p_\nu/\overline{\zeta}_\nu)}{\mathrm{Im}\,\zeta_\nu}\,, \quad d_\nu = \frac{\mathrm{Im}\,p_\nu}{\mathrm{Im}\,\zeta_\nu}\,, \tag{3.1.87}$$

where

$$p_\nu = \prod_{\mu\neq\nu} \frac{1}{(1-\zeta_\mu/\zeta_\nu)(1-\overline{\zeta}_\mu/\zeta_\nu)}\,.$$

There follows

$$\rho_0(x;\mathrm{d}\tilde{\lambda}) = \int_{\mathbb{R}} \frac{\mathrm{d}\lambda(t)}{(x-t)\tilde{\omega}_m(t)} = \sum_\nu \int_{\mathbb{R}} \frac{1}{x-t}\,\frac{c_\nu + d_\nu t}{(t+1/\zeta_\nu)(t+1/\overline{\zeta}_\nu)}\,\mathrm{d}\lambda(t).$$

Here, we can write

$$\frac{1}{x-t}\,\frac{c_\nu + d_\nu t}{(t+1/\zeta_\nu)(t+1/\overline{\zeta}_\nu)} = \frac{A_\nu}{x-t} + \frac{B_\nu}{t+1/\zeta_\nu} + \frac{C_\nu}{t+1/\overline{\zeta}_\nu}\,,$$

where

$$A_\nu = \frac{c_\nu + d_\nu x}{|x+1/\zeta_\nu|^2}\,, \quad B_\nu = \frac{\mathrm{i}}{2\mathrm{Im}(1/\zeta_\nu)}\,\frac{c_\nu - d_\nu/\zeta_\nu}{x+1/\zeta_\nu}\,, \quad C_\nu = \overline{B}_\nu, \tag{3.1.88}$$

to get

$$\rho_0(x;\mathrm{d}\tilde{\lambda}) = \sum_\nu \left(A_\nu \rho_0(x;\mathrm{d}\lambda) - 2\mathrm{Re}[B_\nu \rho_0(-1/\zeta_\nu;\mathrm{d}\lambda)]\right). \tag{3.1.89}$$

Both terms in the sum can again be computed as indicated immediately after (3.1.85). For an application of this procedure, see Example 3.36 of §3.1.4.3.

Example 3.33 Example 3.32, revisited, with $\omega = 0.001$.

The difficult pole here is the one at $-\omega$. The Cauchy integral $\rho_0(x;\mathrm{d}\lambda)$ for $\mathrm{d}\lambda(t) = t^{-1/2}\,\mathrm{d}t$ on $[0,1]$ and $x<0$, required in the two occurrences on the right of (3.1.85), can be obtained in closed form. Indeed,

$$\rho_0(x;\mathrm{d}\lambda) = \int_0^1 \frac{t^{-1/2}\,\mathrm{d}t}{x-t} = -\int_0^1 \frac{t^{-1/2}\,\mathrm{d}t}{|x|+t} \quad (x<0),$$

and the transformation $t=s^2$ in the last integral on the right gives

$$\begin{aligned}\rho_0(x;\mathrm{d}\lambda) &= -\int_0^1 \frac{s^{-1}\cdot 2s\,\mathrm{d}s}{|x|+s^2} = -\frac{2}{|x|}\int_0^1 \frac{\mathrm{d}s}{1+s^2/|x|} \\ &= -\frac{2}{|x|}\int_0^{1/\sqrt{|x|}} \frac{\sqrt{|x|}\,\mathrm{d}t}{1+t^2} = -\frac{2}{\sqrt{|x|}}\tan^{-1}\left(\frac{1}{\sqrt{|x|}}\right).\end{aligned}$$

There follows from (3.1.85), in which $x=-\omega$, that

$$\rho_0(x;\mathrm{d}\tilde{\lambda}) = \rho_0(x;\mathrm{d}\lambda) = -\frac{2}{\sqrt{|x|}}\,\tan^{-1}\left(\frac{1}{\sqrt{|x|}}\right) \quad \text{if } m = 1,$$

$$\rho_0(x;\mathrm{d}\tilde{\lambda}) = \sum_{\nu=1}^{m-1} \frac{2c_\nu}{1+\xi_\nu x}\left\{-\frac{1}{\sqrt{|x|}}\,\tan^{-1}\left(\frac{1}{\sqrt{|x|}}\right) + \sqrt{\xi_\nu}\,\tan^{-1}\sqrt{\xi_\nu}\right\} \quad \text{if } m > 1, \tag{3.1.90}$$

where c_ν is given by (3.1.84). When $m = 1$, the benign poles are ignored and only the difficult one is taken into account. When $m > 2$ is large, the second relation in (3.1.90) is vulnerable to serious cancellation errors, since the constants c_ν can assume large values of either sign; see, in this connection, Gautschi (1993a, p. 124). No such problem occurs when $m = 2$, the summation in (3.1.90) then consisting of just one term.

The procedure is implemented in the `OPQ` routine `Example3_33.m` and was run for $\omega = 0.001$, $m = 2n$, $m = n$, $m = 2$, $m = 1$, and $m = 0$. In the first three cases, the results are quite similar, those for $m = 2$ being slightly more accurate than the others. The latter are shown in Table 3.3 together with the results for the last two cases. Note from the relatively small values of `Ncap` the ease with

Table 3.3 *The integral of Example 3.32 with* $\omega = 0.001$ *evaluated by rational Gauss quadrature.*

n	m	Integral	Error	`Ncap`	`kount`
1	2	96.5045731403309	2.059(–03)	13	8
4	2	96.7036881308250	1.019(–09)	17	4
7	2	96.7036882293812	2.939(–16)	22	3
1	1	96.2844423124649	4.335(–03)	—	—
4	1	96.7036780981287	1.048(–07)	—	—
7	1	96.7036882291188	2.713(–12)	—	—
1	0	5.34185151487088	9.448(–01)	—	—
4	0	23.4324747952258	7.577(–01)	—	—
7	0	39.9488620667821	5.869(–01)	—	—

which accurate results can be obtained when $m > 1$. As expected, this is in stark contrast with the extremely poor answers furnished by the ordinary Gauss formulae ($m = 0$). We also note the benefit accrued from the special treatment of the pole at $-\omega$. Without it, the routine `r_mod.m` would have to work much harder. In the case $m = 2n$, $n = 7$, for example, it returns `Ncap`=351.

Suppose now that we have two difficult poles $\pm x$ outside the support of $\mathrm{d}\lambda$. Then, in place of (3.1.82), the modified measure is

$$\mathrm{d}\hat{\lambda}(t) = \frac{\mathrm{d}\tilde{\lambda}(t)}{t^2 - x^2}\,,$$

and we need to compute its recurrence coefficients $\hat{\alpha}_k$ and $\hat{\beta}_k$. This is the last problem discussed in §2.4.5 and is solved by Algorithm 2.11. It again requires the Cauchy integral (3.1.83) in the combinations $\rho_0(x;\mathrm{d}\tilde{\lambda}) + \rho_0(-x;\mathrm{d}\tilde{\lambda})$ and $\rho_0(x;\mathrm{d}\tilde{\lambda}) - \rho_0(-x;\mathrm{d}\tilde{\lambda})$, or, by virtue of (3.1.85), the Cauchy integrals $\rho_0(\pm x;\mathrm{d}\lambda)$ (in addition to $\rho_0(-1/\xi_\nu;\mathrm{d}\lambda)$ corresponding to the $m-2$ benign poles).

Example 3.34 Example 3.31, revisited, with $\omega = 1.001$.

There is a pair, $\pm\omega$, of difficult poles, and correspondingly $\xi_{1,2} = \pm 1/\omega$ in (3.1.81). The remaining (benign) poles do not necessarily have to be accounted for to high precision. Since $\omega \approx 1$, we can, therefore, replace $\xi_{\nu+2}$ in (3.1.81) by

$$\tilde{\xi}_\nu = \frac{(-1)^\nu}{\lfloor(\nu+3)/2\rfloor}\,, \quad \nu = 1, 2, \ldots, m-2,$$

and define $\tilde{\omega}_m(t) = \prod_{\nu=1}^{m-2}(1+\tilde{\xi}_\nu t)$ (=1 if $m = 2$). We then have (approximately)

$$\omega_m(t) = \left(1 - \frac{1}{\omega^2}\,t^2\right)\tilde{\omega}_m(t) = -\frac{1}{\omega^2}\,(t^2-\omega^2)\tilde{\omega}_m(t),$$

so that the modified measure is

$$\mathrm{d}\hat{\lambda}(t) = \frac{\mathrm{d}t}{\omega_m(t)} = -\omega^2\frac{\mathrm{d}t}{(t^2-\omega^2)\tilde{\omega}_m(t)} = -\omega^2\frac{\mathrm{d}\tilde{\lambda}(t)}{t^2-\omega^2}\,,$$

and Algorithm 2.11 is applicable with $x = \omega$. The required Cauchy integrals

Table 3.4 *The integral of Example 3.31 with* $\omega = 1.001$ *evaluated by rational Gauss quadrature.*

n	m	Integral	Error	`Ncap`	`kount`
1	2	7.60900373691843	4.115(–01)	—	—
4	8	12.9292490747847	6.014(–07)	25	5
7	14	12.9292568506327	4.873(–11)	29	4
1	4	9.41774621137573	2.716(–01)	15	9
4	4	12.9291016962906	1.200(–05)	25	5
7	4	12.9292568467483	2.517(–10)	29	4
1	2	7.60900373691843	4.115(–01)	—	—
4	2	12.9270894147078	1.676(–04)	—	—
7	2	12.9292560307169	6.337(–08)	—	—

$\rho_0(\pm x;\mathrm{d}\tilde{\lambda})$ are given by (3.1.85) and (3.1.84), where the ξ_ν are to be replaced by $\tilde{\xi}_\nu$ and where $\rho_0(x;\mathrm{d}\lambda) = \rho_0(x;\mathrm{d}t)$ is computable explicitly. There follows

$$\begin{aligned}\rho_0(x;\mathrm{d}\tilde{\lambda}) &= \rho_0(x;\mathrm{d}t) = \log\left|\frac{x+1}{x-1}\right| \quad \text{if } m=2,\\ \rho_0(x;\mathrm{d}\tilde{\lambda}) &= \sum_{\nu=1}^{m-2}\frac{c_\nu}{1+\tilde{\xi}_\nu x}\log\left|\frac{(x+1)(\tilde{\xi}_\nu+1)}{(x-1)(\tilde{\xi}_\nu-1)}\right| \quad \text{if } m>2.\end{aligned} \tag{3.1.91}$$

This is implemented in the `OPQ` routine `Example3_34.m`, which for $\omega = 1.001$ and $m = 2n$, $m = 4$, and $m = 2$, produces results as shown in Table 3.4. Note that for the last value of m, only the difficult poles, and none of the benign poles, are incorporated.

3.1.4.3 *Fermi–Dirac and Bose–Einstein integrals* These are integrals of interest in solid state physics when Fermi–Dirac and Bose–Einstein distributions are involved. We consider here generalized versions of these integrals containing an extra parameter θ related to temperature.

Example 3.35 Generalized Fermi–Dirac integral

$$F_k(\eta,\theta) = \int_0^\infty \frac{t^k\sqrt{1+\theta t/2}}{\mathrm{e}^{-\eta+t}+1}\,\mathrm{d}t, \quad \eta\in\mathbb{R},\ \theta\geq 0.$$

Here, k is the Boltzmann constant whose values of physical interest are the half-integers $k = \frac{1}{2}$, $k = \frac{3}{2}$, and $k = \frac{5}{2}$. The parameter η, which can be positive or negative, is a "degeneracy parameter" (Pichon, 1989).

For numerical purposes, it is convenient to write the integral in the form

$$F_k(\eta,\theta) = \int_0^\infty \frac{\sqrt{1+\theta t/2}}{\mathrm{e}^{-\eta}+\mathrm{e}^{-t}}\,t^k\mathrm{e}^{-t}\,\mathrm{d}t, \tag{3.1.92}$$

which suggests the generalized Laguerre measure (cf. Table 1.1) $\mathrm{d}\lambda(t) = t^k\mathrm{e}^{-t}\,\mathrm{d}t$ as the appropriate measure of integration. The poles of the integrand are all simple and occur in conjugate complex pairs on the line $\mathrm{Im}\,\zeta = \eta$ at odd integer multiples of π away from the real axis. All these poles are benign. We are in the case of Example 3.27 and thus take m even and

$$\zeta_\mu = -\frac{1}{\eta+\mu\mathrm{i}\pi}\,,\ \zeta_{\mu+1} = -\frac{1}{\eta-\mu\mathrm{i}\pi}\,, \quad \mu(\text{odd}) = 1,3,\ldots,m-1,$$

that is, in the notation of Example 3.27,

$$\xi_\nu = \frac{-\eta}{\eta^2+(2\nu-1)^2\pi^2}\,,\ \eta_\nu = \frac{(2\nu-1)\pi}{\eta^2+(2\nu-1)^2\pi^2}\,, \quad \nu = 1,2,\ldots,m/2.$$

This gives rise to the positive polynomial ω_m shown in Example 3.27. The n-point rational Gauss formula for (3.1.92) can now be computed as described in the paragraph preceding Example 3.31.

The procedure is implemented in the `OPQ` routine `fermi_dirac.m` and was run for $\theta = 10^{-4}$, $\eta = \pm 1$, and the three values of k, using $m = 2n$, $m = 2\lfloor (n+1)/2\rfloor$,

Table 3.5 *The Fermi–Dirac integral (3.1.92) for* $\eta = -1$, $k = \frac{1}{2}$, *and* $\theta = 10^{-4}$, *evaluated by rational Gauss quadrature.*

n	m	Integral	Error	`Ncap`	`kount`
1	2	0.275409029983064	5.199(–02)	43	15
4	8	0.290512275644047	4.866(–07)	73	10
7	14	0.290512417018931	1.933(–12)	85	8
10	20	0.290512417019493	1.720(–15)	101	7
1	2	0.275409029983064	5.199(–02)	43	15
4	4	0.290512392000444	8.612(–08)	73	10
7	8	0.290512417019499	2.102(–14)	85	8
10	10	0.290512417019493	5.733(–16)	101	7
1	2	0.275409029983064	5.199(–02)	43	15
4	2	0.290512145362808	9.351(–07)	73	10
7	2	0.290512416447331	1.970(–09)	85	8
10	2	0.290512417025901	2.206(–11)	101	7
1	0	0.301304326552001	3.715(–02)	—	—
4	0	0.290442503440480	2.407(–04)	—	—
7	0	0.290513664399923	4.294(–06)	—	—
10	0	0.290512463028434	1.584(–07)	—	—

$m = 2$, and $m = 0$. Table 3.5 shows the results for $k = \frac{1}{2}$, $\eta = -1$, which are typical. It can be seen that the second choice of m, as in Example 3.32, yields slightly more accurate answers than the first, and significantly better accuracy than the other choices of m; see the routine `Example3_35.m` for implementational details. To determine the (relative) errors, we used a quadruple-precision Fortran routine to generate reference values to 24 decimal digits.

Example 3.36 Generalized Bose–Einstein integral

$$G_k(\eta, \theta) = \int_0^\infty \frac{t^k \sqrt{1 + \theta t/2}}{\mathrm{e}^{-\eta + t} - 1} \, \mathrm{d}t, \quad \eta < 0, \ \theta \geq 0.$$

The values of k of interest are the same half-integers $k = \frac{1}{2}$, $k = \frac{3}{2}$, and $k = \frac{5}{2}$ as in Example 3.35, but η now has to be negative.

For numerical work, we choose to write

$$G_k(\eta, \theta) = \int_0^\infty \frac{t\sqrt{1 + \theta t/2}}{\mathrm{e}^{-\eta} - \mathrm{e}^{-t}} \, t^{k-1} \mathrm{e}^{-t} \, \mathrm{d}t, \tag{3.1.93}$$

where a factor t is split off to make the integrand regular at $t = 0$ even in the case $\eta = 0$ (which, however, is excluded). The measure of integration, therefore, is $\mathrm{d}\lambda(t) = t^{k-1}\mathrm{e}^{-t} \, \mathrm{d}t$.

There are again infinitely many simple conjugate complex poles on the line $\mathrm{Im}\,\zeta = \eta$, now at a distance of multiples of 2π away from the real axis. This makes them even more benign than the poles in Example 3.35. There is, however, an additional real pole at $t = \eta$. We are, thus, in the case of Example 3.29, which suggests to take $m \geq 3$ odd, and to put

$$\zeta_\mu = -\frac{1}{\eta + (\mu+1)\mathrm{i}\pi}\,, \quad \zeta_{\mu+1} = -\frac{1}{\eta - (\mu+1)\mathrm{i}\pi}\,, \quad \mu(\mathrm{odd}) = 1, 3, \ldots, m-2,$$

$$\zeta_m = -\frac{1}{\eta}\,.$$

Therefore, in the notation of Example 3.29,

$$\xi_\nu = \frac{-\eta}{\eta^2 + 4\nu^2\pi^2}\,, \quad \eta_\nu = \frac{2\nu\pi}{\eta^2 + 4\nu^2\pi^2}\,, \quad \nu = 1, 2, \ldots, (m-1)/2. \tag{3.1.94}$$

The rational Gauss quadrature rule appropriate for (3.1.93) can be generated

Table 3.6 *The Bose–Einstein integral (3.1.93) evaluated by rational Gauss quadrature.*

n	m	Integral	Error	`Ncap`	`kount`
1	1	0.284309031568454	2.512(–01)	91	20
4	7	0.379707663443525	3.167(–06)	121	13
7	13	0.379708865993066	1.319(–11)	155	11
10	19	0.379708865998074	5.848(–16)	141	9
1	1	0.284309031568454	2.512(–01)	91	20
4	3	0.379708550494209	8.309(–07)	121	13
7	7	0.379708865998149	1.981(–13)	155	11
10	9	0.379708865998074	7.310(–16)	141	9
1	1	0.284309031568454	2.512(–01)	91	20
4	1	0.379698902772340	2.624(–05)	121	13
7	1	0.379708897989683	8.425(–08)	155	11
10	1	0.379708865562790	1.146(–09)	141	9
1	0	0.419669711250205	1.052(–01)	—	—
4	0	0.381220851941995	3.982(–03)	—	—
7	0	0.379832656726223	3.260(–04)	—	—
10	0	0.379725201927930	4.302(–05)	—	—

in the same manner as in Example 3.35, provided $|\eta|$ is not very small. The procedure is implemented in the `OPQ` routine `bose_einstein.m` and used in the routine `Example3_36.m` to obtain the results shown in Table 3.6 for $\theta = 10^{-4}$, $\eta = -1$, $k = \frac{1}{2}$. For the other values of k, the results are similar. Since m, if

positive, should be odd, we took $m = 2n-1$, $m = 2\lfloor (n+1)/2 \rfloor - 1$, $m = 1$, and $m = 0$.

For very small values of $|\eta|$, the real pole at $t = \eta$ must be treated separately as described in §3.1.4.2. According to Example 3.29, we have

$$\omega_m(t) = (1 - t/\eta)\tilde{\omega}_m(t), \quad \tilde{\omega}_m(t) = \prod_{\nu=1}^{(m-1)/2} [(1+\xi_\nu t)^2 + \eta_\nu^2 t^2], \tag{3.1.95}$$

hence

$$\mathrm{d}\hat{\lambda}(t) = \frac{\mathrm{d}\lambda(t)}{\omega_m(t)} = \frac{\mathrm{d}\tilde{\lambda}(t)}{1 - t/\eta} = -\eta \frac{\mathrm{d}\tilde{\lambda}(t)}{t - \eta}\,.$$

Algorithm 2.8 is thus applicable with $x = \eta$. To compute the Cauchy integral $\rho_0(x; \mathrm{d}\tilde{\lambda})$ in (3.1.89), we need the partial fraction decomposition of $\tilde{\omega}_m^{-1}$ in (3.1.86). Since $|\eta|$ is very small, we can simplify (3.1.94) by letting $\xi_\nu \approx \tilde{\xi}_\nu$, $\eta_\nu \approx \tilde{\eta}_\nu$, where

$$\tilde{\xi}_\nu = 0, \quad \tilde{\eta}_\nu = \frac{1}{2\nu\pi}\,, \quad \nu = 1, 2, \ldots, (m-1)/2, \tag{3.1.96}$$

and redefining $\tilde{\omega}_m$ in (3.1.95) by replacing ξ_ν and η_ν by $\tilde{\xi}_\nu$ and $\tilde{\eta}_\nu$, respectively. This makes $\tilde{\omega}_m$ independent of η. An elementary computation based on (3.1.87) and (3.1.88), and using the approximations (3.1.96), then yields

$$\begin{aligned}
\rho_0(x; \mathrm{d}\tilde{\lambda}) &= \rho_0(x; \mathrm{d}\lambda) \quad \text{if } m = 1, \\
\rho_0(x; \mathrm{d}\tilde{\lambda}) &= \sum_{\mu=1}^{(m-1)/2} \frac{2\mu\pi p_\mu}{x^2 + 4\mu^2\pi^2} \, (2\mu\pi\rho_0(x; \mathrm{d}\lambda) \\
&\qquad -\mathrm{Re}[(2\mu\pi - \mathrm{i}x)\rho_0(2\mu\pi\mathrm{i}; \mathrm{d}\lambda)]) \quad \text{if } m \geq 3,
\end{aligned}$$

where

$$p_\mu = \prod_{\substack{\kappa=1 \\ \kappa \neq \mu}}^{(m-1)/2} \frac{\kappa^2}{\kappa^2 - \mu^2}\,.$$

The Cauchy integrals $\rho_0(2\mu\pi\mathrm{i}; \mathrm{d}\lambda)$ are computable by the continued fraction algorithm of §2.3.2, which converges rapidly. The same algorithm applied to $\rho_0(x; \mathrm{d}\lambda)$, when $x < 0$ is close to zero, would converge very slowly. Fortunately, we can compute $\rho_0(x; \mathrm{d}\lambda)$ analytically. Indeed,

$$\rho_0(x; \mathrm{d}\lambda) = \int_0^\infty \frac{t^{k-1}\mathrm{e}^{-t}}{x - t}\,\mathrm{d}t = -\int_0^\infty \frac{t^{k-1}\mathrm{e}^{-t}}{|x| + t}\,\mathrm{d}t,$$

and by the change of variables $t \mapsto |x|t$,

$$\rho_0(x;\mathrm{d}\lambda) = -|x|^{k-1}\int_0^\infty \frac{t^{k-1}\mathrm{e}^{-|x|t}}{1+t}\,\mathrm{d}t.$$

The integral on the right is expressible in terms of the incomplete gamma function as $\Gamma(k)\mathrm{e}^{|x|}\Gamma(1-k,|x|) = \Gamma(k)\mathrm{e}^{|x|}\{\Gamma(1-k)-\gamma(1-k,|x|)\}$ (see Gradshteyn and Ryzhik (2000, eqn 3.383.10)), which, upon using $\Gamma(k)\Gamma(1-k) = \pi/\sin(\pi k)$ and the power series expansion of $\gamma(1-k,|x|)$, yields

$$\rho_0(x;\mathrm{d}\lambda) = -\mathrm{e}^{|x|}\left(\frac{\pi}{\sin(\pi k)}\,|x|^{k-1} - \Gamma(k)\sum_{j=0}^{\infty}(-1)^j\frac{|x|^j}{(j+1-k)j!}\right).$$

The series on the right converges quite rapidly when $|x|$ is small. The procedure is impemented in the `OPQ` procedure `bose_einstein_diffpole.m`.

Example 3.37 Example 3.36, revisited, with $\eta = -0.001$.

Here, the pole at $t = \eta$ is clearly difficult, calling for the procedure embodied in the routine `bose_einstein_diffpole.m`. The results produced by this routine, when $\theta = 10^{-4}$ and the m are chosen as in Example 3.36, are displayed in Table 3.7 for the case $k = \frac{1}{2}$. The other values of k yield similar results, although not quite as bad when $m = 0$; see the routine `Example3_37.m`. The integers `Ncap` and `kount` characterize, as before, the computer intensity of the discretization

Table 3.7 *The Bose–Einstein integral (3.1.93) with* $\eta = -0.001$ *evaluated by rational Gauss quadrature.*

n	m	Integral	Error	`Ncap`	`kount`	`nu1`
1	1	1.69040669641165	2.376(–01)	—	—	—
4	7	2.21714386900473	2.811(–06)	49	8	30
7	13	2.21715010087722	1.543(–11)	71	7	30
1	1	1.69040669641165	2.376(–01)	—	—	—
4	3	2.21714726128018	1.281(–06)	49	8	30
7	7	2.21715010090452	3.110(–12)	71	7	30
1	1	1.69040669641165	2.376(–01)	—	—	—
4	1	2.21713613862449	6.297(–06)	—	—	—
7	1	2.21714956475764	2.418(–07)	—	—	—
1	0	2.24665592228785	1.331(–02)	—	—	—
4	0	2.30358500893463	3.899(–02)	—	—	—
7	0	2.29973499254897	3.725(–02)	—	—	—

procedure in the routine `mcdis.m` for generating the recurrence coefficients of the (partially) modified measure $\mathrm{d}\tilde{\lambda} = \mathrm{d}\lambda/\tilde{\omega}_m$. Table 3.7 shows in addition the integer `nu1`, which is related to the computation of the Cauchy integral $\rho_0(2\mu\pi\mathrm{i};\mathrm{d}\lambda)$ for $\mu = 1$, indicating the integer ν required for the continued fraction algorithm

(2.3.14) to converge. Since all complex poles are benign, and the argument $2\mu\pi$i in the Cauchy integral is comfortably far away from the real axis, neither `Ncap` nor `nu1` are particularly large. Note that in the case $m = 1$, only the real pole at $t = \eta$ is taken into account.

All the numerical illustrations, so far, used the rather small value of $\theta = 10^{-4}$ taken from the physics literature (Sagar, 1991). The performance of the rational Gauss formulae, as constructed, is bound to deteriorate with increasing θ, on account of the square root singularity at $t = -2/\theta$. To prevent this from happening, one incorporates the factor $s(t) = \sqrt{1 + \theta t/2}$ into the modified measure, as indicated in the Remark to Theorem 3.25. This puts the burden on the discretization procedure in the routine `mcdis.m`, which will have to work harder. But once the respective coefficients $\hat{\alpha}_k(s\mathrm{d}\lambda/\omega_m)$ and $\hat{\beta}_k(s\mathrm{d}\lambda/\omega_m)$ have been generated, the quadrature rule (3.1.80) is readily obtained, and so are the rational Gauss formulae, which now, even for large values of θ, enjoy again the rapid convergence that we have seen in the previous examples. The modification, incidentally, necessitates only one small change in the quadrature routine used by `mcdis.m` (called by `r_mod.m`) and in the function routine evaluating the integrand. (The necessary changes are identified in comments within the routines `quadrat.m` and `fex35.m`, `fex37.m`.) But the effect of these changes can be rather dramatic, as is illustrated in the next example.

Example 3.38 The generalized Fermi–Dirac integral for large θ.

We reran `Example3_35.m`, with the changes noted above, for $\theta = 1$, $\theta = 10$, and $\theta = 100$. In the last case, the error tolerance `eps0` was lowered from $10^2\times$`eps` to $10^6\times$`eps`$= 2.22 \times 10^{-10}$ in order to ease the burden on the routine `mcdis.m`. The results for $\eta = -1$, $k = \frac{1}{2}$ are shown in Table 3.8. Note the large values of `Ncap` that are required, but the good accuracies achieved. The last column, in contrast, shows the errors incurred when no changes are incorporated.

Table 3.8 *The Fermi–Dirac integral (3.1.92) for large θ.*

θ	n	m	Integral	Error	`Ncap`	`kount`	Error0
1.0	1	2	0.361184320447425	5.910(–02)	51	16	9.834(–02)
	4	8	0.383869494230472	7.153(–07)	73	10	1.439(–06)
	7	14	0.383869768810864	3.325(–12)	85	8	7.033(–09)
10.0	1	2	0.769108163428219	6.228(–02)	251	27	1.247(–01)
	4	8	0.820187855482118	8.348(–07)	265	18	4.588(–04)
	7	14	0.820188540206230	4.059(–12)	351	16	6.872(–05)
100.0	1	2	2.2667230470	6.191(–02)	571	33	1.249(–01)
	4	8	2.4163266837	8.397(–07)	617	24	1.791(–03)
	7	14	2.4163287128	1.499(–11)	743	21	5.367(–04)

The same treatment is applicable in the case of Bose–Einstein integrals with similar results. The case $\theta = 100$, however, proved to strain the routine `mcdis.m`

more than before, and the error tolerance `eps0` had to be reduced some more to $10^7 \times$`eps`$=2.22\times10^{-9}$ to achieve convergence within the limit `Nmax`$=1000$ of the discretization parameter N. The results for $\eta = -1$, $k = \frac{1}{2}$ are shown in Table 3.9; they were produced by a slightly changed routine `Example3_36.m`. (The specific changes are indicated in comment lines.)

Table 3.9 *The Bose–Einstein integral (3.1.93) for large θ.*

θ	n	m	Integral	Error	`Ncap`	`kount`	Error0
1.0	1	1	.354699024506360	2.725(–01)	91	20	3.720(–01)
	4	7	.487528382100474	4.623(–06)	121	13	1.445(–05)
	7	13	.487530635992235	2.280(–11)	155	11	1.418(–08)
10.0	1	1	.722916404688393	2.799(–01)	283	28	5.436(–01)
	4	7	1.00386348178076	5.524(–06)	265	18	8.699(–04)
	7	13	1.00386902658501	2.871(–11)	351	16	1.140(–04)
100.0	1	1	2.1604929294	2.606(–01)	763	35	5.991(–01)
	4	7	2.9219317372	5.484(–06)	745	25	3.033(–03)
	7	13	2.9219477618	4.323(–11)	743	21	8.530(–04)

3.1.4.4 *Rational Gauss–Radau and Gauss–Lobatto formulae* The discussion of §3.1.4.1 for rational Gauss formulae extends almost verbatim to Gauss–Radau and Gauss–Lobatto formulae. It suffices, therefore, to simply state the respective facts, referring to eqn (3.1.71) for the definition of the space $\mathbb{Q}_m$ and to eqn (3.1.75) for the definition of the polynomial ω_m.

With regard to the "left-handed" Gauss–Radau formula

$$\int_{\mathbb{R}} f(t)\,\mathrm{d}\lambda(t) = \lambda_0 f(a) + \sum_{\nu=1}^{n} \lambda_\nu f(\tau_\nu) + R_n(f), \tag{3.1.97}$$

where $a = \inf \operatorname{supp}(\mathrm{d}\lambda)$, we now assume, in place of (3.1.70), that

$$0 \le m \le 2n+1, \tag{3.1.98}$$

and the appropriate rational/polynomial space is

$$\mathbb{S}_{2n+1} = \mathbb{Q}_m \oplus \mathbb{P}_{2n-m}. \tag{3.1.99}$$

We then have the following characterization of rational Gauss–Radau formulae.

Theorem 3.39 *Given the integer m satisfying (3.1.98), assume that the measure $\mathrm{d}\lambda/\omega_m$ admits an $(n+1)$-point Gauss–Radau formula*

$$\int_{\mathbb{R}} p(t)\frac{\mathrm{d}\lambda(t)}{\omega_m(t)} = \lambda_0^R p(a) + \sum_{\nu=1}^{n} \lambda_\nu^R p(\tau_\nu^R) \quad \textit{for all } p \in \mathbb{P}_{2n}, \tag{3.1.100}$$

with distinct internal nodes τ_ν^R in the open support interval (a,b) of $\mathrm{d}\lambda$. If $\mathbb{S}_{2n+1}$ is defined by (3.1.99), then

$$\tau_\nu = \tau_\nu^R, \quad \lambda_\nu = \lambda_\nu^R \omega_m(\tau_\nu^R), \quad \nu = 0, 1, 2, \ldots, n, \tag{3.1.101}$$

yields formula (3.1.97) exact for $f \in \mathbb{S}_{2n+1}$.

There is, of course, an analogous result for "right-handed" Gauss–Radau formulae.

For Gauss–Lobatto formulae,

$$\int_{\mathbb{R}} f(t)\,\mathrm{d}\lambda(t) = \lambda_0 f(a) + \sum_{\nu=1}^{n} \lambda_\nu f(\tau_\nu) + \lambda_{n+1} f(b) + R_n(f), \tag{3.1.102}$$

we assume

$$0 \le m \le n + 2 \tag{3.1.103}$$

and define the space

$$\mathbb{S}_{2n+2} = \mathbb{Q}_m \oplus \mathbb{P}_{2n+1-m}. \tag{3.1.104}$$

Theorem 3.40 *Given the integer* m *satisfying (3.1.103), assume that the measure* $\mathrm{d}\lambda/\omega_m$ *admits an* $(n+2)$*-point Gauss–Lobatto formula*

$$\int_{\mathbb{R}} p(t)\frac{\mathrm{d}\lambda(t)}{\omega_m(t)} = \lambda_0^L p(a) + \sum_{\nu=1}^{n} \lambda_\nu^L p(\tau_\nu^L) + \lambda_{n+1}^L p(b) \quad \textit{for all } p \in \mathbb{P}_{2n+1}, \tag{3.1.105}$$

with distinct internal nodes τ_ν^L *in the open support interval* (a, b) *of* $\mathrm{d}\lambda$. *If* $\mathbb{S}_{2n+2}$ *is defined by (3.1.104), then*

$$\tau_\nu = \tau_\nu^L, \quad \lambda_\nu = \lambda_\nu^L \omega_m(\tau_\nu^L), \quad \nu = 0, 1, \ldots, n, n+1, \tag{3.1.106}$$

yields formula (3.1.102) exact for all $f \in \mathbb{S}_{2n+2}$.

For implementations in Matlab, see the `OPQ` routines `radau_rational.m` and `lobatto_rational.m`.

3.1.4.5 *Rational Gauss–Kronrod formulae* Recall that a Gauss–Kronrod formula for the measure $\mathrm{d}\lambda$ has the form (cf. (3.1.39))

$$\int_{\mathbb{R}} f(t)\,\mathrm{d}\lambda(t) = \sum_{\nu=1}^{n} \lambda_\nu f(\tau_\nu) + \sum_{\mu=1}^{n+1} \lambda_\mu^* f(\tau_\mu^*) + R_n(f), \tag{3.1.107}$$

where τ_ν are the Gauss nodes for $\mathrm{d}\lambda$, and the remaining nodes τ_μ^* and all the weights are such that $R_n(f) = 0$ for all $f \in \mathbb{P}_{3n+1}$. To make the formula exact on a rational/polynomial space, one defines an integer m with

$$0 \le m \le 3n + 2, \tag{3.1.108}$$

and the space

$$\mathbb{S}_{3n+2} = \mathbb{Q}_m \oplus \mathbb{P}_{3n+1-m}, \tag{3.1.109}$$

where $\mathbb{Q}_m$ is defined by (3.1.71). If the polynomial ω_m is defined as in (3.1.75), then, exactly as in §3.1.4.1, one proves the following theorem.

Theorem 3.41 *Given the integer m satisfying (3.1.108), assume that the measure $\mathrm{d}\lambda/\omega_m$ admits a $(2n+1)$-point Gauss–Kronrod formula*

$$\int_{\mathbb{R}} p(t)\frac{\mathrm{d}\lambda(t)}{\omega_m(t)} = \sum_{\nu=1}^{n} \lambda_\nu^K p(\tau_\nu^G) + \sum_{\mu=1}^{n+1} \lambda_\mu^{*K} p(\tau_\mu^K) \quad \textit{for all } p \in \mathbb{P}_{3n+1}, \tag{3.1.110}$$

having distinct nodes τ_ν^G and $\tau_\mu^K \neq \tau_\nu^G$ contained in the support interval $[a,b]$ of $\mathrm{d}\lambda$. If $\mathbb{S}_{3n+2}$ is defined by (3.1.109), then

$$\begin{aligned} \tau_\nu = \tau_\nu^G,\ \tau_\mu^* = \tau_\mu^K;\quad \lambda_\nu = \lambda_\nu^K \omega_m(\tau_\nu^G),\ \lambda_\mu^* = \lambda_\mu^{*K}\omega_m(\tau_\mu^K), \\ \nu = 1,2,\ldots,n;\ \mu = 1,2,\ldots,n+1, \end{aligned} \tag{3.1.111}$$

yields formula (3.1.107) exact for all $f \in \mathbb{S}_{3n+2}$.

Recall from §3.1.2.1 that τ_ν^G in (3.1.110) are the zeros of the orthogonal polynomial $\pi_n(\,\cdot\,;\mathrm{d}\lambda/\omega_m)$ and τ_μ^K the zeros of the Stieltjes polynomial $\pi_{n+1}^K(\,\cdot\,;\mathrm{d}\lambda/\omega_m)$. The procedure implied by Theorem 3.41 is embodied in the `OPQ` routine `kronrod_rational.m`.

Example 3.42 Example 3.31, revisited.

The integral of Example 3.31 is now evaluated by the rational Gauss–Kronrod quadrature rule generated according to Theorem 3.41. This is done by the `OPQ` routine `Example3_42.m`, the core of which looks very similar to the one exhibited in Example 3.31:

```
ab0=r_jacobi(Nmax);
eps0=100*eps; sgn=1;
for m=1:M
   sgn=-sgn;
   Z(m,1)=sgn/(om*floor((m+1)/2)); Z(m,2)=1;
end
[abmod,Ncap,kount]=r_mod(ceil(3*N/2)+1,ab0);
xw=kronrod_rational(N,abmod);
```

The results obtained for the same value $\omega = 1.1$ as in Table 3.1 and for $m = 2\lfloor(3n+2)/2\rfloor$, $m = 2n$, $m = 2\lfloor(n+1)/2\rfloor$, $m = 2$ are displayed in Table 3.10. For comparison, we also include the results for $m = 0$ corresponding to ordinary Gauss–Kronrod quadrature. Compared to ordinary or rational Gauss rules (Table 3.1) as well as to ordinary Gauss–Kronrod rules ($m = 0$ in Table 3.10), the improvement provided by the rational Gauss–Kronrod rule is rather spectacular, even if only the first pair of poles ($m = 2$) is incorporated.

3.1.4.6 *Rational Gauss–Turán formulae* For the Gauss–Turán formula (cf. (3.1.58))

$$\int_{\mathbb{R}} f(t)\,\mathrm{d}\lambda(t) = \sum_{\nu=1}^{n}\sum_{\sigma=0}^{2s} \lambda_\nu^{(\sigma)} f^{(\sigma)}(\tau_\nu) + R_{n,s}(f), \tag{3.1.112}$$

Table 3.10 *The integral of Example 3.31 with* $\omega = 1.1$ *evaluated by rational Gauss–Kronrod quadrature.*

n	m	Integral	Error	`Ncap`	`kount`
1	4	4.46666779324154	2.475(–04)	43	9
2	8	4.46777619256081	5.699(–07)	49	8
3	10	4.46777364646169	1.655(–11)	61	7
4	14	4.46777364638776	1.193(–15)	57	6
1	2	4.46120976114983	1.469(–03)	43	9
2	4	4.46780896475528	7.905(–06)	49	8
3	6	4.46777364819601	4.047(–10)	61	7
4	8	4.46777364638719	1.290(–13)	57	6
5	10	4.46777364638776	1.590(–15)	73	6
1	2	4.46120976114983	1.469(–03)	43	9
2	2	4.46816030252371	8.654(–05)	49	8
3	4	4.46777366865229	4.983(–09)	61	7
4	4	4.46777364631047	1.730(–11)	57	6
5	6	4.46777364638776	1.590(–15)	73	6
1	2	4.46120976114983	1.469(–03)	43	9
3	2	4.46777488157599	2.765(–07)	61	7
5	2	4.46777364637416	3.044(–12)	73	6
7	2	4.46777364638776	1.392(–15)	73	5
1	0	3.95672776447190	1.144(–01)	—	—
4	0	4.46883197103820	2.369(–04)	—	—
7	0	4.46779291459554	4.313(–06)	—	—
10	0	4.46777387752509	5.173(–08)	—	—

we assume

$$0 \le m \le 2(s+1)n \tag{3.1.113}$$

and define

$$\mathbb{S}_{2(s+1)n} = \mathbb{Q}_m \oplus \mathbb{P}_{2(s+1)n-m-1}, \tag{3.1.114}$$

where $\mathbb{Q}_m$ is the space of rationals defined in (3.1.71). (We trust the reader will not confuse the running index s used in (3.1.71) with the s in the Gauss–Turán formula (3.1.112).) Our objective is to make (3.1.112) exact on the space $\mathbb{S}_{2(s+1)n}$ in (3.1.114). If $m = 0$, this gives the classical Gauss–Turán formula exact for all polynomials of degree $\le 2(s+1)n - 1$ (cf. §3.1.3.1). Let again ω_m be defined by (3.1.75). The following theorem provides the answer to our objective.

Theorem 3.43 *Given the integer* m *satisfying (3.1.113), assume that the measure* $\mathrm{d}\lambda/\omega_m$ *admits a Gauss–Turán formula*

$$\int_{\mathbb{R}} p(t)\frac{\mathrm{d}\lambda(t)}{\omega_m(t)} = \sum_{\nu=1}^{n}\sum_{\sigma=0}^{2s} \lambda_\nu^{(\sigma)T} p^{(\sigma)}(\tau_\nu^T) \quad \textit{for all } p \in \mathbb{P}_{2(s+1)n-1}, \tag{3.1.115}$$

having distinct nodes τ_ν^T *contained in the support interval* $[a,b]$ *of* $\mathrm{d}\lambda$. *If* $\mathbb{S}_{2(s+1)n}$ *is defined as in (3.1.114), then*

$$\begin{aligned} &\tau_\nu = \tau_\nu^T, \quad \nu = 1,2,\ldots,n, \\ &\lambda_\nu^{(\sigma)} = \sum_{\rho=\sigma}^{2s} \lambda_\nu^{(\rho)T} \binom{\rho}{\sigma} \omega_m^{(\rho-\sigma)}(\tau_\nu^T), \\ &\qquad\qquad \nu = 1,2,\ldots,n;\ \sigma = 0,1,\ldots,2s, \end{aligned} \tag{3.1.116}$$

yields formula (3.1.112) exact for all $f \in \mathbb{S}_{2(s+1)n}$.

Proof To prove exactness on $\mathbb{S}_{2(s+1)n}$, let f be an arbitrary element of this space. Then, either $f \in \mathbb{Q}_m$ or $f \in \mathbb{P}_{2(s+1)n-m-1}$. In either case, $\omega_m f \in \mathbb{P}_{2(s+1)n-1}$. Indeed, in the former case we have, say, $f(t) = (1+\zeta_\mu t)^{-r}$, so that $\omega_m f \in \mathbb{P}_{m-r}$, and since $m \le 2(s+1)n$ by (3.1.113), and $r \ge 1$, the assertion follows. In the other case, it follows trivially. Consequently, by (3.1.115),

$$\int_{\mathbb{R}} f(t)\,\mathrm{d}\lambda(t) = \int_{\mathbb{R}} \omega_m(t) f(t) \frac{\mathrm{d}\lambda(t)}{\omega_m(t)} = \sum_{\nu=1}^{n}\sum_{\rho=0}^{2s} \lambda_\nu^{(\rho)T} (\omega_m f)^{(\rho)}(\tau_\nu^T).$$

Applying Leibniz's rule of differentiation, and then interchanging the order of summation, we obtain for the inner sum

$$\begin{aligned} &\sum_{\rho=0}^{2s} \lambda_\nu^{(\rho)T} \sum_{\sigma=0}^{\rho} \binom{\rho}{\sigma} \omega_m^{(\rho-\sigma)}(\tau_\nu^T) f^{(\sigma)}(\tau_\nu^T) \\ &\quad = \sum_{\sigma=0}^{2s} f^{(\sigma)}(\tau_\nu^T) \sum_{\rho=\sigma}^{2s} \lambda_\nu^{(\rho)T} \binom{\rho}{\sigma} \omega_m^{(\rho-\sigma)}(\tau_\nu^T) \\ &\quad = \sum_{\sigma=0}^{2s} \lambda_\nu^{(\sigma)} f^{(\sigma)}(\tau_\nu), \end{aligned}$$

the last expression by definition of $\lambda_\nu^{(\sigma)}$ and τ_ν in (3.1.116). Summing over ν yields (3.1.112) with zero remainder term. □

The computation of $\lambda_\nu^{(\sigma)}$ in (3.1.116) requires successive derivatives of ω_m. They can be obtained as follows. Let

$$s_k(t) = \sum_{\mu=1}^{m} \left(\frac{\zeta_\mu}{1+\zeta_\mu t}\right)^k$$

and note that

$$s_k'(t) = -k s_{k+1}(t).$$

From

$$\frac{\omega_m'(t)}{\omega_m(t)} = \sum_{\mu=1}^{m} \frac{\zeta_\mu}{1+\zeta_\mu t} = s_1(t),$$

that is, $\omega_m' = s_1\omega_m$, repeated differentiation then yields

$$\begin{aligned}
\omega_m'' &= s_1'\omega_m + s_1\omega_m' = -s_2\omega_m + s_1 \cdot s_1\omega_m = (-s_2 + s_1^2)\omega_m,\\
\omega_m''' &= (-s_2' + 2s_1s_1')\omega_m + (-s_2 + s_1^2)s_1\omega_m\\
&= (2s_3 - 2s_1s_2)\omega_m + (-s_1s_2 + s_1^3)\omega_m\\
&= (2s_3 - 3s_1s_2 + s_1^3)\omega_m,\\
\omega_m'''' &= (2s_3' - 3s_1's_2 - 3s_1s_2' + 3s_1^2s_1')\omega_m + (2s_3 - 3s_1s_2 + s_1^3)s_1\omega_m\\
&= (-6s_4 + 3s_2^2 + 6s_1s_3 - 3s_1^2s_2)\omega_m + (2s_1s_3 - 3s_1^2s_2 + s_1^4)\omega_m\\
&= (-6s_4 + 8s_1s_3 + 3s_2^2 - 6s_1^2s_2 + s_1^4)\omega_m,
\end{aligned}$$

etc.

For an illustration of the rational Gauss–Turán formula as applied to the integral of Example 3.31, see Gautschi, Gori, and Lo Cascio (2000, Example 2.2).

3.1.5 *Cauchy principal value integrals*

In analogy to (2.3.1), we define the *Cauchy principal value integral* of a function f by

$$(\mathcal{C}f)(x;\mathrm{d}\lambda) = \int\!\!\!\!\!\!-_{\mathbb{R}} \frac{f(t)}{x-t}\,\mathrm{d}\lambda(t), \tag{3.1.117}$$

where $\mathrm{d}\lambda$ is a positive measure supported on an interval $[a,b]$, $-\infty \le a < b \le \infty$, and x is an interior point of $[a,b]$. It is possible to adapt Gaussian quadrature rules to evaluating Cauchy principal value integrals of the form (3.1.117). In principle, one may distinguish between two types of quadrature rules: one in which x appears as a node, and one in which it does not. In the former case, the quadrature rule has the form

$$(\mathcal{C}f)(x;\mathrm{d}\lambda) = c_0(x)f(x) + \sum_{\nu=1}^{n} c_\nu(x)f(\tau_\nu) + R_n(f;x), \tag{3.1.118}$$

and in the latter case the form

$$(\mathcal{C}f)(x;\mathrm{d}\lambda) = \sum_{\nu=1}^{n} c_\nu^*(x)f(\tau_\nu^*) + R_n^*(f;x). \tag{3.1.119}$$

In either case, the nodes τ_ν and τ_ν^* are assumed independent of x. We call (3.1.118) a *modified quadrature rule*, and (3.1.119) a *quadrature rule in the strict*

sense. The two rules have essentially different character: formula (3.1.118) can be made "Gaussian," that is, to have degree of exactness $2n$, whereas (3.1.119) cannot. In fact, the degree of exactness of (3.1.119) cannot exceed $n-1$, since otherwise $(\mathcal{C}f)(x;\mathrm{d}\lambda) \equiv 0$ when $f(t) = \prod_{\nu=1}^{n}(t-\tau_\nu^*)$, which contradicts a well-known inversion formula for Cauchy principal value integrals (cf. Gakhov (1990, §42.3); Muskhelishvili (1977, §86)). We discuss the two types of quadrature rules separately.

3.1.5.1 *Modified Gauss quadrature formula* The basic idea is to write (3.1.117) in the form

$$(\mathcal{C}f)(x;\mathrm{d}\lambda) = f(x)\int\!\!\!\!\!\!-_{\mathbb{R}} \frac{\mathrm{d}\lambda(t)}{x-t} - \int_{\mathbb{R}} \frac{f(x)-f(t)}{x-t}\,\mathrm{d}\lambda(t) \tag{3.1.120}$$

and to apply the n-point Gauss quadrature rule (1.4.7) to the second integral on the right. If we observe from (1.3.40) and (1.4.8), by letting $z \to x$ in these formulae, that

$$\int\!\!\!\!\!\!-_{\mathbb{R}} \frac{\mathrm{d}\lambda(t)}{x-t} = \frac{\rho_n(x)}{\pi_n(x)} + \sum_{\nu=1}^{n} \frac{\lambda_\nu^G}{x-\tau_\nu^G},$$

where $\rho_n(x)$ is defined by (2.3.6), then the result is

$$(\mathcal{C}f)(x;\mathrm{d}\lambda) = \frac{\rho_n(x)}{\pi_n(x)}\,f(x) + \sum_{\nu=1}^{n} \lambda_\nu^G \frac{f(\tau_\nu^G)}{x-\tau_\nu^G} + R_n(f;x). \tag{3.1.121}$$

This is exact whenever $f \in \mathbb{P}_{2n}$. Note from (1.4.9) and (1.3.40) that

$$\lambda_\nu^G = -\frac{\rho_n(\tau_\nu^G)}{\pi_n'(\tau_\nu^G)}, \quad \nu = 1,2,\ldots,n. \tag{3.1.122}$$

We remark that (3.1.121) and (3.1.122) remain valid if τ_ν^G and λ_ν^G are replaced by nodes and weights of any interpolatory quadrature rule and π_n by the respective node polynomial, except that the degree of exactness will be correspondingly smaller. In particular, therefore, we may construct for (3.1.117) modified versions of the Gauss–Radau, Gauss–Lobatto, etc., quadrature rules.

Since π_n' has opposite signs at two consecutive zeros τ_ν^G and $\tau_{\nu+1}^G$ of π_n, it follows by (3.1.122) and $\lambda_\nu^G > 0$ that the same is true for ρ_n. Thus, *between any two consecutive zeros of* π_n*, there is at least one zero of* ρ_n. If x is a zero of ρ_n, formula (3.1.121) becomes particularly noteworthy,

$$\int\!\!\!\!\!\!-_{\mathbb{R}} \frac{f(t)}{x-t}\,\mathrm{d}\lambda(t) = \sum_{\nu=1}^{n} \lambda_\nu^G \frac{f(\tau_\nu^G)}{x-\tau_\nu^G} + R_n(f;x) \quad (\rho_n(x)=0). \tag{3.1.123}$$

This is just the Gauss formula applied to the integral on the left, as if it were an ordinary integral! An instance of (3.1.123) occurs if $\mathrm{d}\lambda$ is a *symmetric* measure (cf. Definition 1.16). Then π_n, for n even, is an even polynomial by Theorem 1.17,

and consequently $\rho_n(0) = 0$. Thus, (3.1.123) becomes applicable with $x = 0$, and we obtain the pretty formula

$$⨍_{\mathbb{R}} \frac{f(t)}{t}\,\mathrm{d}\lambda(t) = \sum_{\nu=1}^{n} \lambda_\nu^G \frac{f(\tau_\nu^G)}{\tau_\nu^G} - R_n(f;0) \quad (\mathrm{d}\lambda \text{ symmetric, } n \text{ even}), \tag{3.1.124}$$

a formula that is also exact whenever $f \in \mathbb{P}_{2n}$.

On the other hand, as x approaches one of the nodes τ_ν^G, the first term on the right of (3.1.121) becomes infinite and, therefore, since $(\mathcal{C}f)(\tau_\nu^G;\mathrm{d}\lambda)$ is finite, a term in the summation of (3.1.121) must also tend to infinity, but with opposite sign. This means that for x near a node τ_ν^G, the numerical use of (3.1.121) is subject to severe cancellation error. Similar difficulties occur with quadrature rules in the strict sense, as will be seen in the next subsection. They can be overcome by organizing the computation in a different way. This will be discussed in 3.1.5.3.

3.1.5.2 *Gauss quadrature formula in the strict sense* A formula of the type (3.1.119) can be obtained by approximating f in (3.1.117) by the polynomial of degree $\leq n-1$ interpolating f at the nodes τ_ν^G,

$$f(t) = p_{n-1}(f;t) + E_{n-1}(f;t), \quad p_{n-1}(f;t) = \sum_{\nu=1}^{n} \frac{\pi_n(t)}{(t-\tau_\nu^G)\pi_n'(\tau_\nu^G)}\, f(\tau_\nu^G),$$

where $E_{n-1}(f;t) \equiv 0$ if $f \in \mathbb{P}_{n-1}$. Integration then yields

$$(\mathcal{C}f)(x;\mathrm{d}\lambda) = \sum_{\nu=1}^{n} \frac{f(\tau_\nu^G)}{\pi_n'(\tau_\nu^G)} ⨍_{\mathbb{R}} \frac{\pi_n(t)}{(x-t)(t-\tau_\nu^G)}\,\mathrm{d}\lambda(t) + R_n^*(f;x),$$

where $R_n^*(f;x) = ⨍_{\mathbb{R}} E_{n-1}(f;t)\mathrm{d}\lambda(t)/(x-t)$. Here we write

$$\frac{1}{(x-t)(t-\tau_\nu^G)} = \frac{1}{x-\tau_\nu^G}\left(\frac{1}{x-t} + \frac{1}{t-\tau_\nu^G}\right)$$

and obtain the desired quadrature rule in the form

$$(\mathcal{C}f)(x;\mathrm{d}\lambda) = \sum_{\nu=1}^{n} \frac{\rho_n(x) - \rho_n(\tau_\nu^G)}{\pi_n'(\tau_\nu^G)(x-\tau_\nu^G)}\, f(\tau_\nu^G) + R_n^*(f;x). \tag{3.1.125}$$

By construction, it has degree of exactness $n-1$, and as was observed earlier, this is the maximum degree possible, unless $\rho_n(x) = 0$, in which case (3.1.125) reduces to (3.1.123) by virtue of (3.1.122). Written in the form (3.1.125), the quadrature rule is again subject to cancellation errors when x is near τ_ν^G.

3.1.5.3 *Computational considerations* Formulae (3.1.121) and (3.1.125) are often used as a means of discretization, for example in the context of singular

integral equations. For the purpose of simply evaluating Cauchy principal value integrals, it may be better to rework these formulae because of the cancellation problems mentioned. The quadrature sums in question indeed can be evaluated in a stable manner for any x in the support interval of $\mathrm{d}\lambda$ by writing them in a different manner. We first show this for formula (3.1.125).

We expand $p_{n-1}(f;\,\cdot\,)$ in the orthogonal polynomials π_k,

$$p_{n-1}(f;t) = \sum_{k=0}^{n-1} a_k \pi_k(t). \tag{3.1.126}$$

By Theorem 1.22 and the fact that $p_{n-1}(f;\tau_\nu^G) = f(\tau_\nu^G)$, we have

$$a_k = \frac{1}{\|\pi_k\|_{\mathrm{d}\lambda}^2} \sum_{\nu=1}^{n} \lambda_\nu^G \pi_k(\tau_\nu^G) f(\tau_\nu^G).$$

Integration of (3.1.126) in the sense of (3.1.117) then yields

$$(\mathcal{C}f)(x;\mathrm{d}\lambda) = \sum_{k=0}^{n-1} a_k \rho_k(x) + R_n^*(f;x). \tag{3.1.127}$$

Recall from §2.3.1 that $\rho_k(x)$ can be computed from the basic three-term recurrence relation (2.3.4),

$$\rho_{k+1}(x) = (x-\alpha_k)\rho_k(x) - \beta_k \rho_{k-1}(x), \quad k = 0, 1, \ldots, n-2, \tag{3.1.128}$$

started with the initial values in (2.3.7),

$$\rho_{-1}(x) = 1, \quad \rho_0(x) = \int_{\mathbb{R}} \frac{\mathrm{d}\lambda(t)}{x-t}\,. \tag{3.1.129}$$

This is an entirely stable procedure, but it requires the Hilbert transform $\rho_0(x)$ of $\mathrm{d}\lambda$. The latter is often available analytically, or can be computed as in Example 2.51.

With regard to formula (3.1.121), we first observe that it, too, can be interpreted as the result of integrating an interpolation polynomial, but now the polynomial of degree $\le n$ that interpolates f at x and the τ_ν^G,

$$\begin{aligned} f(t) &= p_n(f;t) + E_n(f;t), \\ p_n(f;t) &= \frac{\pi_n(t)}{\pi_n(x)}\, f(x) + \sum_{\nu=1}^{n} \frac{(t-x)\pi_n(t)}{(t-\tau_\nu^G)(\tau_\nu^G - x)\pi_n'(\tau_\nu^G)}\, f(\tau_\nu^G). \end{aligned} \tag{3.1.130}$$

Integrating in the sense of (3.1.117) and noting (3.1.122) then, indeed, yields (3.1.121). Therefore, in place of (3.1.126) and (3.1.127), we write

$$p_n(f;t) = \sum_{k=0}^{n} b_k \pi_k(t) \tag{3.1.131}$$

and

$$(\mathcal{C}f)(x;\mathrm{d}\lambda) = \sum_{k=0}^{n} b_k \rho_k(x) + R_n(f;x), \tag{3.1.132}$$

where $R_n(f;x) = \int\!\!\!\!\!\!-_{\mathbb{R}}\ E_n(f;t)\,\mathrm{d}\lambda(t)/(x-t)$. The first n coefficients b_k turn out to be the same as those in (3.1.127). Indeed,

$$b_k = \frac{1}{\|\pi_k\|^2} \int_{\mathbb{R}} p_n(f;t)\pi_k(t)\,\mathrm{d}\lambda(t), \tag{3.1.133}$$

where the integrand, if $k < n$, is a polynomial of degree $\leq 2n-1$. Hence, n-point Gauss quadrature applied to the integral yields

$$b_k = \frac{1}{\|\pi_k\|^2} \sum_{\nu=1}^{n} \lambda_\nu^G f(\tau_\nu^G)\pi_k(\tau_\nu^G) = a_k, \quad k < n, \tag{3.1.134}$$

by virtue of the interpolation property of $p_n(f;\,\cdot\,)$. If $k = n$, we insert in (3.1.133) the expression for $p_n(f;\,\cdot\,)$ from (3.1.130) and obtain

$$b_n = \frac{1}{\|\pi_n\|^2} \int_{\mathbb{R}} \left[\frac{\pi_n(t)}{\pi_n(x)}\, f(x) + \sum_{\nu=1}^{n} \frac{(t-x)\pi_n(t)}{(t-\tau_\nu^G)(\tau_\nu^G - x)\pi_n'(\tau_\nu^G)}\, f(\tau_\nu^G) \right] \pi_n(t)\,\mathrm{d}\lambda(t).$$

Here, we note from the fact that the elementary Lagrange interpolation polynomials sum up to 1 that

$$\frac{1}{\pi_n(x)} = \sum_{\nu=1}^{n} \frac{1}{(x-\tau_\nu^G)\pi_n'(\tau_\nu^G)}\,,$$

and, furthermore, that

$$\frac{1}{\|\pi_n\|^2} \int_{\mathbb{R}} \frac{(t-x)\pi_n(t)}{t-\tau_\nu^G}\, \pi_n(t)\,\mathrm{d}\lambda(t) = 1,$$

since the fraction in the integrand is a monic polynomial of degree n. There follows

$$b_n = \sum_{\nu=1}^{n} \frac{f(x) - f(\tau_\nu^G)}{(x-\tau_\nu^G)\pi_n'(\tau_\nu^G)}\,. \tag{3.1.135}$$

Given any function f, the fraction on the right needs to be evaluated with some care in order to avoid cancellation, but this is less of a problem than in (3.1.125).

We note that the sums in (3.1.127) and in (3.1.132) can be evaluated by Clenshaw's algorithm (cf. §2.1.8.1). The approximations in (3.1.127) and (3.1.132) are incorporated in the `OPQ` routine `cauchyPVI.m` with input parameter `iopt`=1 and `iopt`$\neq$ 1, respectively.

Example 3.44 The Cauchy principal value integral

$$\fint_{-1}^{1} \frac{\cos t}{x-t}\,\mathrm{d}t = \cos x[\mathrm{Ci}(1+x) - \mathrm{Ci}(1-x)] + \sin x[\mathrm{Si}(1+x) + \mathrm{Si}(1-x)],$$

where $-1 < x < 1$ and Ci and Si are the cosine and sine integrals, respectively (cf. Abramowitz and Stegun (1992, eqns 5.2.1 and 5.2.2)).

We applied both (3.1.127) and (3.1.132) with $x = 1/3$ and show the results in Table 3.11. For the computation of the errors, Maple was used to obtain

Table 3.11 *The Cauchy principal value integral of Example 3.44 evaluated by (3.1.127) and (3.1.132).*

n	(3.1.127)	Error	(3.1.132)	Error
2	0.58079622092461	3.954(–01)	0.97612959894783	8.041(–05)
4	0.96503213749523	1.118(–02)	0.97621000982213	1.048(–09)
6	0.97613431261510	7.570(–05)	0.97621001086992	2.220(–16)
9	0.97621001166259	7.927(–10)	—	—
13	0.97621001086992	1.332(–15)	—	—

20-decimal values of the cosine and sine integrals. Convergence is seen to be quite fast, but the exceptionally fast convergence of the modified Gauss quadrature rule (3.1.132) is worth noting. The computation is done in the `OPQ` routine `Example3_44.m`.

3.1.6 *Polynomials orthogonal on several intervals*

The problem we wish to consider here is the following. We are given a finite set of intervals $[c_j, d_j]$, disjoint or not, and on each interval $[c_j, d_j]$ a positive measure $\mathrm{d}\lambda_j$. Define $\mathrm{d}\lambda(t) = \sum_j \chi_{[c_j,d_j]}(t)\,\mathrm{d}\lambda_j(t)$, where $\chi_{[c_j,d_j]}$ is the characteristic function of the interval $[c_j, d_j]$,

$$\chi_{[c_j,d_j]}(t) = \begin{cases} 1 & \text{if } t \in [c_j, d_j], \\ 0 & \text{otherwise.} \end{cases}$$

Assuming the Jacobi matrices $\boldsymbol{J}^{(j)} = \boldsymbol{J}_n(\mathrm{d}\lambda_j)$ for the measures $\mathrm{d}\lambda_j$ to be known, find the Jacobi matrix $\boldsymbol{J} = \boldsymbol{J}_n(\mathrm{d}\lambda)$ for $\mathrm{d}\lambda$. We will give two solutions to this problem, one based on Stieltjes's procedure and the other based on the modified Chebyshev algorithm. Gauss quadrature is an essential tool in both solutions.

3.1.6.1 *Solution by Stieltjes's procedure* In §2.2.3.1, we described Stieltjes's procedure for calculating the recurrence coefficients for polynomials orthogonal relative to a discrete measure. The same algorithm, in principle, works for any measure $\mathrm{d}\lambda$ if there is a good way to calculate the inner products involved. Thus, to recall, one computes α_0 from (1.3.3) for $k = 0$ and β_0 from (1.3.6). Then, the recurrence relation (1.3.2) is used with $k = 0$ to obtain π_1. This allows us to compute α_1 and β_1 from (1.3.3) and (1.3.4) with $k = 1$, and thus π_2 from (1.3.2)

with $k = 1$. Proceeding in this manner, one is able to successively compute all recurrence coefficients $\alpha_k(\mathrm{d}\lambda)$, $\beta_k(\mathrm{d}\lambda)$, $k = 0, 1, \ldots, n-1$, hence the Jacobi matrix $\boldsymbol{J}_n(\mathrm{d}\lambda)$.

Since all inner products that must be calculated in this procedure require integration (with respect to $\mathrm{d}\lambda$) of polynomials of degree $\leq 2n-1$, we can use n-point Gauss quadrature

$$\int_{c_j}^{d_j} p(t)\,\mathrm{d}\lambda_j(t) = \sum_{\nu=1}^{n} \lambda_\nu^{(j)} p(\tau_\nu^{(j)}), \quad p \in \mathbb{P}_{2n-1},$$

for the measure $\mathrm{d}\lambda_j$ on each constituent interval $[c_j, d_j]$ of $\mathrm{d}\lambda$, or else, by virtue of the Remark to Theorem 3.1, the formula

$$\int_{c_j}^{d_j} p(t)\,\mathrm{d}\lambda_j(t) = \beta_0^{(j)} \boldsymbol{e}_1^{\mathrm{T}} p(\boldsymbol{J}^{(j)}) \boldsymbol{e}_1,$$

where $\beta_0^{(j)} = \int_{c_j}^{d_j} \mathrm{d}\lambda_j(t)$. Therefore,

$$\int_{\mathbb{R}} p(t)\,\mathrm{d}\lambda(t) = \sum_j \beta_0^{(j)} \boldsymbol{e}_1^{\mathrm{T}} p(\boldsymbol{J}^{(j)}) \boldsymbol{e}_1, \quad p \in \mathbb{P}_{2n-1}. \tag{3.1.136}$$

This allows us to compute the inner products in Stieltjes's procedure entirely in terms of matrix manipulations involving the Jacobi matrices $\boldsymbol{J}^{(j)}$.

We illustrate this for the inner product

$$(t\pi_k, \pi_k)_{\mathrm{d}\lambda} = \int_{\mathbb{R}} t\pi_k^2(t)\,\mathrm{d}\lambda(t) = \sum_j \int_{c_j}^{d_j} t\pi_k^2(t)\,\mathrm{d}\lambda_j(t). \tag{3.1.137}$$

Define

$$\boldsymbol{\zeta}_k^{(j)} = \pi_k(\boldsymbol{J}^{(j)}) \boldsymbol{e}_1, \quad \boldsymbol{e}_1^{\mathrm{T}} = [1, 0, \ldots, 0] \in \mathbb{R}^n. \tag{3.1.138}$$

Then, by (3.1.137) and (3.1.136),

$$(t\pi_k, \pi_k)_{\mathrm{d}\lambda} = \sum_j \beta_0^{(j)} \boldsymbol{e}_1^{\mathrm{T}} \boldsymbol{J}^{(j)} [\pi_k(\boldsymbol{J}^{(j)})]^2 \boldsymbol{e}_1 = \sum_j \beta_0^{(j)} \boldsymbol{e}_1^{\mathrm{T}} \pi_k(\boldsymbol{J}^{(j)}) \boldsymbol{J}^{(j)} \pi_k(\boldsymbol{J}^{(j)}) \boldsymbol{e}_1,$$

that is,

$$(t\pi_k, \pi_k)_{\mathrm{d}\lambda} = \sum_j \beta_0^{(j)} \boldsymbol{\zeta}_k^{(j)\mathrm{T}} \boldsymbol{J}^{(j)} \boldsymbol{\zeta}_k^{(j)}.$$

Similarly (in fact, a bit simpler), one finds

$$(\pi_k, \pi_k)_{\mathrm{d}\lambda} = \sum_j \beta_0^{(j)} \boldsymbol{\zeta}_k^{(j)\mathrm{T}} \boldsymbol{\zeta}_k^{(j)}.$$

The updating of $\boldsymbol{\zeta}_k^{(j)}$ required in Stieltjes's procedure follows immediately from (1.3.2) and (3.1.138). We summarize as follows.

Algorithm 3.1 (Stieltjes procedure for polynomials orthogonal on several intervals)

Initialization:

$$\boldsymbol{\zeta}_0^{(j)} = \boldsymbol{e}_1, \quad \boldsymbol{\zeta}_{-1}^{(j)} = 0 \quad (\text{all } j),$$
$$\alpha_0 = \frac{\sum_j \beta_0^{(j)} \boldsymbol{e}_1^{\mathrm{T}} \boldsymbol{J}^{(j)} \boldsymbol{e}_1}{\sum_j \beta_0^{(j)}}, \quad \beta_0 = \sum_j \beta_0^{(j)}.$$

Continuation (if $n > 1$): for $k = 0, 1, \ldots, n-2$ do

$$\boldsymbol{\zeta}_{k+1}^{(j)} = (\boldsymbol{J}^{(j)} - \alpha_k \boldsymbol{I})\boldsymbol{\zeta}_k^{(j)} - \beta_k \boldsymbol{\zeta}_{k-1}^{(j)} \quad (\text{all } j),$$
$$\alpha_{k+1} = \frac{\sum_j \beta_0^{(j)} \boldsymbol{\zeta}_{k+1}^{(j)\mathrm{T}} \boldsymbol{J}^{(j)} \boldsymbol{\zeta}_{k+1}^{(j)}}{\sum_j \beta_0^{(j)} \boldsymbol{\zeta}_{k+1}^{(j)\mathrm{T}} \boldsymbol{\zeta}_{k+1}^{(j)}}, \quad \beta_{k+1} = \frac{\sum_j \beta_0^{(j)} \boldsymbol{\zeta}_{k+1}^{(j)\mathrm{T}} \boldsymbol{\zeta}_{k+1}^{(j)}}{\sum_j \beta_0^{(j)} \boldsymbol{\zeta}_k^{(j)\mathrm{T}} \boldsymbol{\zeta}_k^{(j)}}.$$

It can be seen that the basic matrix/vector operations, apart from vector additions, that are required in this algorithm are premultiplication of a vector by a Jacobi matrix and the formation of scalar products.

The `OPQ` routine implementing Algorithm 3.1 is `r_multidomain_sti.m`.

Example 3.45 Example 2.38, revisited.

This is the case of two identical intervals $[-1, 1]$, the first carrying a multiple c of the Legendre and the second the Chebyshev weight function. The combined measure has recurrence coefficients that can be computed either by the multiple-component discretization procedure, as described in Example 2.38, or by the multidomain algorithm described in this section. The Matlab program for the latter looks something like this:

Table 3.12 *The Chebyshev weight function plus a multiple c of the Legendre weight function.*

n	$c = 1$	$c = 10$	$c = 100$
0	5.1415926536	23.1415926536	203.1415926536
1	0.4351692451	0.3559592080	0.3359108398
5	0.2510395775	0.2535184776	0.2528129500
12	0.2500610870	0.2504824840	0.2505324193
25	0.2500060034	0.2500682357	0.2501336338
51	0.2500006590	0.2500082010	0.2500326887
79	0.2500001724	0.2500021136	0.2500127264

```
ab1=r_jacobi(N); ab1(1,2)=2*c;
ab2=r_jacobi(N,-.5);
abmd=[ab1 ab2];
ab=r_multidomain_sti(N,abmd);
```

For the complete program, see the routine `Example3_45.m` with `iopt`=1. The results for $c = 1$, $c = 10$, and $c = 100$, and for selected values of n are shown in Table 3.12. They are in complete agreement (except for one small discrepancy in the last digit) with those in Gautschi (1994, Table VI).

3.1.6.2 *Solution by the modified Chebyshev algorithm* Let p_k be a set of monic polynomials satisfying a three-term recurrence relation

$$p_{k+1}(t) = (t - a_k)p_k(t) - b_k p_{k-1}(t), \quad k = 0, 1, 2, \dots,$$
$$p_0(t) = 1, \quad p_{-1}(t) = 0$$

with known coefficients a_k and b_k, and let

$$m_k = \int_{\mathbb{R}} p_k(t)\, \mathrm{d}\lambda(t), \quad k = 0, 1, 2, \dots,$$

denote the modified moments of $\mathrm{d}\lambda$ relative to the polynomials p_k. The first $2n - 1$ coefficients a_k, b_k, $k = 0, 1, \dots, 2n - 2$, and the first $2n$ moments m_k, $k = 0, 1, \dots, 2n-1$, suffice for Algorithm 2.1, the modified Chebyshev algorithm, to be able to generate the desired recursion coefficients $\alpha_k(\mathrm{d}\lambda)$, $\beta_k(\mathrm{d}\lambda)$, $k = 0, 1, \dots, n - 1$, and with them, the Jacobi matrix $\boldsymbol{J}_n(\mathrm{d}\lambda)$. The choice of the polynomials p_k is at our discretion.

The computation of the modified moments by Gauss quadrature is entirely analogous to the computation of the inner products in §3.1.6.1. One defines

$$z_k^{(j)} = p_k(\boldsymbol{J}^{(j)})\boldsymbol{e}_1$$

and then obtains

$$m_k = \sum_j \beta_0^{(j)} \boldsymbol{z}_k^{(j)\mathrm{T}} \boldsymbol{e}_1.$$

Algorithm 3.2 (Computing the first $2n$ modified moments of $\mathrm{d}\lambda$)
Initialization:

$$\boldsymbol{z}_0^{(j)} = \boldsymbol{e}_1, \quad \boldsymbol{z}_{-1}^{(j)} = \boldsymbol{0} \quad (\text{all } j), \quad m_0 = \sum_j \beta_0^{(j)}.$$

Continuation: for $k = 0, 1, \dots, 2n - 2$ do

$$\boldsymbol{z}_{k+1}^{(j)} = (\boldsymbol{J}^{(j)} - a_k \boldsymbol{I})\boldsymbol{z}_k^{(j)} - b_k \boldsymbol{z}_{k-1}^{(j)},$$
$$m_{k+1} = \sum_j \beta_0^{(j)} \boldsymbol{z}_{k+1}^{(j)\mathrm{T}} \boldsymbol{e}_1.$$

The modified Chebyshev algorithm in conjunction with Algorithm 3.2 is implemented in the `OPQ` routine `r_multidomain_cheb.m`. It was used, employing Legendre moments, to redo Example 3.45, producing results that are identical with those in Table 3.12 but taking about three times as long to run. See `Example3_45.m` with `iopt`$\neq 1$.

3.1.7 *Quadrature estimation of matrix functionals*

Let $\boldsymbol{A} \in \mathbb{R}^{N\times N}$ be a positive definite matrix and f a function analytic on an interval containing the spectrum of $\boldsymbol{A}$. The problem to be considered is to find lower and upper bounds for the bilinear form

$$\boldsymbol{u}^{\mathrm{T}} f(\boldsymbol{A})\boldsymbol{v}, \tag{3.1.139}$$

where $\boldsymbol{u}, \boldsymbol{v} \in \mathbb{R}^N$ are given vectors. At first sight, this seems to be unrelated to quadrature, but on closer inspection it turns out that (3.1.139) can be expressed as an integral of f relative to some (admittedly unknown) discrete measure. This is the key observation that will allow us to solve the problem posed.

Assume for simplicity that $\boldsymbol{A}$ has distinct[5] eigenvalues λ_n,

$$0 < \lambda_N < \lambda_{N-1} < \cdots < \lambda_1, \tag{3.1.140}$$

and denote the respective (orthonormal) eigenvectors by $\boldsymbol{v}_n$,

$$\boldsymbol{A}\boldsymbol{v}_n = \lambda_n \boldsymbol{v}_n, \quad \boldsymbol{v}_n^{\mathrm{T}}\boldsymbol{v}_m = \delta_{nm}, \quad n, m = 1, 2, \ldots, N.$$

(We trust the reader will not confuse these λs with the weights in the Gauss quadrature rule (3.1.1).) Then, we have the spectral decomposition of $\boldsymbol{A}$,

$$\boldsymbol{A}\boldsymbol{V} = \boldsymbol{V}\boldsymbol{\Lambda}, \quad \boldsymbol{\Lambda} = \boldsymbol{V}^{\mathrm{T}}\boldsymbol{A}\boldsymbol{V}, \tag{3.1.141}$$

where $\boldsymbol{V} = [\boldsymbol{v}_1, \boldsymbol{v}_2, \ldots, \boldsymbol{v}_N]$, $\boldsymbol{\Lambda} = \operatorname{diag}(\lambda_1, \lambda_2, \ldots, \lambda_N)$. If we assume, for the moment, that $\boldsymbol{u} = \boldsymbol{v}$ in (3.1.139), we put

$$\boldsymbol{u} = \sum_{k=1}^{N} \rho_k \boldsymbol{v}_k, \tag{3.1.142}$$

where for simplicity (cf. footnote) $\rho_k \neq 0$, all k. Then, $\boldsymbol{u} = \boldsymbol{V}\boldsymbol{\rho}$, where $\boldsymbol{\rho} = [\rho_1, \rho_2, \ldots, \rho_N]^{\mathrm{T}}$, and from (3.1.141) we have $f(\boldsymbol{A}) = \boldsymbol{V} f(\boldsymbol{\Lambda})\boldsymbol{V}^{\mathrm{T}}$, so that

$$\boldsymbol{u}^{\mathrm{T}} f(\boldsymbol{A})\boldsymbol{u} = \boldsymbol{\rho}^{\mathrm{T}}\boldsymbol{V}^{\mathrm{T}}\boldsymbol{V} f(\boldsymbol{\Lambda})\boldsymbol{V}^{\mathrm{T}}\boldsymbol{V}\boldsymbol{\rho} = \boldsymbol{\rho}^{\mathrm{T}} f(\boldsymbol{\Lambda})\boldsymbol{\rho}.$$

Thus,

$$\boldsymbol{u}^{\mathrm{T}} f(\boldsymbol{A})\boldsymbol{u} = \sum_{k=1}^{N} \rho_k^2 f(\lambda_k) =: \int_{\mathbb{R}_+} f(t)\,\mathrm{d}\rho_N(t), \tag{3.1.143}$$

where $\mathrm{d}\rho_N$ is the discrete measure supported on the eigenvalues λ_k of $\boldsymbol{A}$ and having positive jumps ρ_k^2 at λ_k. Without loss of generality we may assume that $\|\boldsymbol{u}\| = 1$, where $\|\cdot\|$ is the Euclidean vector norm; then,

$$\int_{\mathbb{R}_+} \mathrm{d}\rho_N(t) = 1. \tag{3.1.144}$$

[5]Otherwise, some terms in (3.1.142) consolidate, so that N becomes smaller.

The case $\boldsymbol{u} \neq \boldsymbol{v}$ can be handled by using, for example, the polarization identity

$$\boldsymbol{u}^{\mathrm{T}} f(\boldsymbol{A})\boldsymbol{v} = \tfrac{1}{4}(\boldsymbol{p}^{\mathrm{T}} f(\boldsymbol{A})\boldsymbol{p} - \boldsymbol{q}^{\mathrm{T}} f(\boldsymbol{A})\boldsymbol{q}), \tag{3.1.145}$$

where $\boldsymbol{p} = \boldsymbol{u} + \boldsymbol{v}$, $\boldsymbol{q} = \boldsymbol{u} - \boldsymbol{v}$. Applying appropriate bounds to the two terms on the right yields bounds for the term on the left.

We also observe that the assumption of positive definiteness for $\boldsymbol{A}$ can be lifted and replaced by nonsingularity in the special (but important) case $f(t) = t^{-1}$. It suffices to note that

$$\boldsymbol{u}^{\mathrm{T}} \boldsymbol{A}^{-1} \boldsymbol{v} = \boldsymbol{u}^{\mathrm{T}} (\boldsymbol{A}^{\mathrm{T}} \boldsymbol{A})^{-1} \boldsymbol{w} \quad \text{with} \quad \boldsymbol{w} = \boldsymbol{A}^{\mathrm{T}} \boldsymbol{v}. \tag{3.1.146}$$

If there is a simple method to generate the orthogonal polynomials relative to $\mathrm{d}\rho_N$ or, equivalently, the Jacobi matrix $\boldsymbol{J}_N(\mathrm{d}\rho_N)$, then the desired bounds for (3.1.143) can be obtained by appropriate Gauss-type quadrature rules (for examples, see §3.1.7.2). One such method is Lanczos's algorithm.

3.1.7.1 *Lanczos's algorithm* Let $\boldsymbol{v}_1, \boldsymbol{v}_2, \ldots, \boldsymbol{v}_N$, as in (3.1.141), be the normalized eigenvectors of the matrix $\boldsymbol{A}$, and let $\boldsymbol{h}_0$ be a given vector of unit length, represented in the basis of eigenvectors as

$$\boldsymbol{h}_0 = \sum_{k=1}^{N} \rho_k \boldsymbol{v}_k, \quad \|\boldsymbol{h}_0\| = 1. \tag{3.1.147}$$

Let $\mathrm{d}\rho_N$ be the discrete measure in (3.1.143) with jumps ρ_k^2, the squares of the ρ_k in (3.1.147). Lanczos's algorithm is a procedure that allows us to generate the orthonormal polynomials $\tilde{\pi}_k(\,\cdot\,; \mathrm{d}\rho_N)$, $k = 0, 1, \ldots, N-1$, or else, the Jacobi matrix $\boldsymbol{J}_N(\mathrm{d}\rho_N)$, entirely by matrix–vector multiplications involving the matrix $\boldsymbol{A}$. It is defined as follows.

Algorithm 3.3 (Lanczos algorithm)

Initialization:

$$\boldsymbol{h}_0 \text{ prescribed with } \|\boldsymbol{h}_0\| = 1, \quad \boldsymbol{h}_{-1} = \boldsymbol{0}.$$

Continuation: for $j = 0, 1, \ldots, N-1$ do

$$\begin{aligned}
\alpha_j &= \boldsymbol{h}_j^{\mathrm{T}} \boldsymbol{A} \boldsymbol{h}_j, \\
\tilde{\boldsymbol{h}}_{j+1} &= (\boldsymbol{A} - \alpha_j \boldsymbol{I})\boldsymbol{h}_j - \gamma_j \boldsymbol{h}_{j-1}, \\
\gamma_{j+1} &= \|\tilde{\boldsymbol{h}}_{j+1}\|, \\
\boldsymbol{h}_{j+1} &= \tilde{\boldsymbol{h}}_{j+1}/\gamma_{j+1}.
\end{aligned}$$

Note that γ_0 can be arbitrary (it multiplies $\boldsymbol{h}_{-1} = \boldsymbol{0}$), but, in accordance with (3.1.144), is often defined by $\gamma_0 = 1$.

The vectors $\boldsymbol{h}_0, \boldsymbol{h}_1, \ldots, \boldsymbol{h}_N$ are called *Lanczos vectors*. They enjoy the following properties, as can be checked by induction.

1. The Lanczos vectors are mutually orthonormal.
2. The vectors $\{\boldsymbol{h}_j\}_{j=0}^n$, $n < N$, form an orthonormal basis of the *Krylov space*
$$\mathcal{K}_n(\boldsymbol{A}, \boldsymbol{h}_0) = \operatorname{span}(\boldsymbol{h}_0, \boldsymbol{A}\boldsymbol{h}_0, \ldots, \boldsymbol{A}^n \boldsymbol{h}_0).$$
3. There holds
$$\boldsymbol{h}_j = p_j(\boldsymbol{A})\boldsymbol{h}_0, \quad j = 0, 1, \ldots, N, \tag{3.1.148}$$
where p_j is a polynomial of degree j satisfying the three-term recurrence relation
$$\begin{aligned} \gamma_{j+1} p_{j+1}(\lambda) &= (\lambda - \alpha_j) p_j(\lambda) - \gamma_j p_{j-1}(\lambda), \\ & \qquad\qquad j = 0, 1, \ldots, N-1, \\ p_0(\lambda) &= 1, \quad p_{-1}(\lambda) = 0. \end{aligned} \tag{3.1.149}$$

We claim that $p_k(\,\cdot\,) = \tilde{\pi}_k(\,\cdot\,; \mathrm{d}\rho_N)$. Indeed, from (3.1.141) one has

$$p_n(\boldsymbol{\Lambda}) = \boldsymbol{V}^{\mathrm{T}} p_n(\boldsymbol{A}) \boldsymbol{V};$$

hence, by (3.1.148),

$$\boldsymbol{h}_n = \boldsymbol{V} p_n(\boldsymbol{\Lambda}) \boldsymbol{V}^{\mathrm{T}} \boldsymbol{h}_0.$$

Orthonormality $\boldsymbol{h}_n^{\mathrm{T}} \boldsymbol{h}_m = \delta_{nm}$ of the Lanczos vectors $\boldsymbol{h}_j$ then yields

$$\boldsymbol{h}_0^{\mathrm{T}} \boldsymbol{V} p_n(\boldsymbol{\Lambda}) \boldsymbol{V}^{\mathrm{T}} \boldsymbol{V} p_m(\boldsymbol{\Lambda}) \boldsymbol{V}^{\mathrm{T}} \boldsymbol{h}_0 = \boldsymbol{h}_0^{\mathrm{T}} \boldsymbol{V} p_n(\boldsymbol{\Lambda}) p_m(\boldsymbol{\Lambda}) \boldsymbol{V}^{\mathrm{T}} \boldsymbol{h}_0 = \delta_{nm}.$$

Since, by (3.1.147), $\boldsymbol{V}^{\mathrm{T}} \boldsymbol{h}_0 = \sum_{k=1}^N \rho_k \boldsymbol{e}_k$, with $\boldsymbol{e}_k$ the kth coordinate vector, one gets

$$\begin{aligned} &\sum_{k,\ell=1}^N \rho_k \boldsymbol{e}_k^{\mathrm{T}} \operatorname{diag}(p_n(\lambda_1) p_m(\lambda_1), \ldots, p_n(\lambda_N) p_m(\lambda_N)) \rho_\ell \boldsymbol{e}_\ell \\ &= \sum_{k,\ell=1}^N \rho_k \rho_\ell \boldsymbol{e}_k^{\mathrm{T}} p_n(\lambda_\ell) p_m(\lambda_\ell) \boldsymbol{e}_\ell = \sum_{k=1}^N \rho_k^2 p_n(\lambda_k) p_m(\lambda_k) = \delta_{nm}, \end{aligned}$$

as claimed.

The recurrence relation (3.1.149), therefore, must be identical with the one in Theorem 1.29 for $\mathrm{d}\lambda = \mathrm{d}\rho_N$, that is, $\gamma_j = \sqrt{\beta_j}$.

If the measure $\mathrm{d}\rho_N$ is not normalized, and one puts as usual

$$\beta_0 = \int_{\mathbb{R}_+} \mathrm{d}\rho_N(t), \tag{3.1.150}$$

the recurrence relation (3.1.149) continues to hold, except that one must define $p_0(\lambda) = 1/\sqrt{\beta_0}$.

3.1.7.2 *Examples* We illustrate the techniques proposed in this section with two examples.

Example 3.46 Error bounds for linear algebraic systems.

Consider the system of linear algebraic equations

$$\boldsymbol{A}\boldsymbol{x} = \boldsymbol{b}, \tag{3.1.151}$$

where $\boldsymbol{A} \in \mathbb{R}^{N\times N}$ is symmetric and positive definite. Given an approximation $\boldsymbol{x}^*$ to the exact solution $\boldsymbol{x} = \boldsymbol{A}^{-1}\boldsymbol{b}$, we wish to estimate the error $\boldsymbol{x} - \boldsymbol{x}^*$ in some norm, say the Euclidean vector norm $\|\cdot\|$.

Since $\boldsymbol{x}^*$ is known, we can compute the residual $\boldsymbol{r}$ of $\boldsymbol{x}^*$,

$$\boldsymbol{r} = \boldsymbol{b} - \boldsymbol{A}\boldsymbol{x}^*. \tag{3.1.152}$$

From $\boldsymbol{x} - \boldsymbol{x}^* = \boldsymbol{A}^{-1}\boldsymbol{r}$ and the symmetry of $\boldsymbol{A}$, it then follows immediately that

$$\|\boldsymbol{x} - \boldsymbol{x}^*\|^2 = \boldsymbol{r}^{\mathrm{T}}\boldsymbol{A}^{-2}\boldsymbol{r}.$$

This is a functional of the type (3.1.143), with $\boldsymbol{u} = \boldsymbol{r}$ and $f(t) = t^{-2}$, and, therefore,

$$\|\boldsymbol{x} - \boldsymbol{x}^*\|^2 = \int_{\mathbb{R}_+} t^{-2}\,\mathrm{d}\rho_N(t). \tag{3.1.153}$$

The discrete orthonormal polynomials belonging to the measure $\mathrm{d}\rho_N$ can be generated by Lanczos's algorithm applied with

$$\boldsymbol{h}_0 = \boldsymbol{r}/\|\boldsymbol{r}\|.$$

Hence, we have access to the Gauss-type quadrature rules of §3.1.1 with $\mathrm{d}\lambda = \mathrm{d}\rho_N$ and are in the fortunate situation of the derivatives of $f(t) = t^{-2}$ being of constant sign on $\mathbb{R}_+$, namely

$$f^{(2n)}(t) > 0, \quad f^{(2n+1)}(t) < 0 \quad \text{for } t \in \mathbb{R}_+. \tag{3.1.154}$$

It then follows from Corollary to Theorem 1.48 that n-point Gauss quadrature (with $n < N$) applied to the integral in (3.1.153) yields a lower bound for the squared error $\|\boldsymbol{x} - \boldsymbol{x}^*\|^2$. Likewise, by Theorems 3.3 and 3.7, if the spectrum of $\boldsymbol{A}$ can be enclosed in an interval $[a, b]$, $0 < a < b$, the "left-handed" $(n+1)$-point Gauss–Radau formula (3.1.13) and the $(n+2)$-point Gauss–Lobatto formula (3.1.26) yield upper bounds, and the "right-handed" formula (3.1.21) a lower bound for (3.1.153).

Analogous results hold for the A-norm $\|\boldsymbol{u}\|_A^2 = \boldsymbol{u}^{\mathrm{T}}\boldsymbol{A}\boldsymbol{u}$, since then

$$\|\boldsymbol{x} - \boldsymbol{x}^*\|_A^2 = \boldsymbol{r}^{\mathrm{T}}\boldsymbol{A}^{-1}\boldsymbol{r},$$

and $f(t) = t^{-1}$ satifies the same inequalities as in (3.1.154).

Example 3.47 Diagonal elements of the inverse of a matrix.

Let $\boldsymbol{A} \in \mathbb{R}^{N\times N}$ be positive definite. The problem is to find bounds for the diagonal elements $(\boldsymbol{A}^{-1})_{ii}$ of $\boldsymbol{A}^{-1}$, $i = 1, 2, \ldots, N$.

Here, we have

$$(\boldsymbol{A}^{-1})_{ii} = \boldsymbol{e}_i^{\mathrm{T}} \boldsymbol{A}^{-1} \boldsymbol{e}_i,$$

where $\boldsymbol{e}_i$ is the ith coordinate vector. This is (3.1.143) with $\boldsymbol{u} = \boldsymbol{e}_i$ and $f(t) = t^{-1}$, and we are in the case mentioned at the end of the previous example. Hence, Gauss-type quadrature rules again provide lower and upper bounds. The Jacobi matrix $\boldsymbol{J}_n = \boldsymbol{J}_n(\mathrm{d}\rho_N)$ required for generating these rules can be obtained by Lanczos's algorithm applied with $\boldsymbol{h}_0 = \boldsymbol{e}_i$.

In the case of the n-point Gauss formula, using the Remark to Theorem 3.1 and noting that $\beta_0 = 1$, we obtain

$$(\boldsymbol{A}^{-1})_{ii} = \int_{\mathbb{R}_+} t^{-1}\, \mathrm{d}\rho_N(t) > \boldsymbol{e}_1^{\mathrm{T}} \boldsymbol{J}_n^{-1} \boldsymbol{e}_1, \quad \boldsymbol{e}_1^{\mathrm{T}} = [1, 0, \ldots, 0] \in \mathbb{R}^n. \tag{3.1.155}$$

Let us use this for $n = 2$. We apply two steps of the Lanczos algorithm with $\boldsymbol{h}_0 = \boldsymbol{e}_i$ to compute

$$\boldsymbol{J}_2 = \begin{bmatrix} \alpha_0 & \gamma_1 \\ \gamma_1 & \alpha_1 \end{bmatrix}.$$

According to Algorithm 3.3, we have

$$\begin{aligned}
&\alpha_0 = a_{ii},\\
&\tilde{\boldsymbol{h}}_1 = (\boldsymbol{A} - \alpha_0 \boldsymbol{I})\boldsymbol{e}_i = [a_{1i}, \ldots, a_{i-1,i}, 0, a_{i+1,i}, \ldots, a_{Ni}]^{\mathrm{T}},\\
&\gamma_1 = \sqrt{\sum_{k\neq i} a_{ki}^2} =: s_i,\\
&\boldsymbol{h}_1 = \tilde{\boldsymbol{h}}_1 / s_i,\\
&\alpha_1 = \frac{1}{s_i^2}\, \tilde{\boldsymbol{h}}_1^{\mathrm{T}} \boldsymbol{A} \tilde{\boldsymbol{h}}_1 = \frac{1}{s_i^2} \sum_{k\neq i} \sum_{\ell \neq i} a_{k\ell} a_{ki} a_{\ell i}.
\end{aligned} \tag{3.1.156}$$

Since

$$\boldsymbol{J}_2^{-1} = \frac{1}{\alpha_0\alpha_1 - \gamma_1^2} \begin{bmatrix} \alpha_1 & -\gamma_1 \\ -\gamma_1 & \alpha_0 \end{bmatrix},$$

one has

$$\boldsymbol{e}_1^{\mathrm{T}} \boldsymbol{J}_2^{-1} \boldsymbol{e}_1 = \frac{\alpha_1}{\alpha_0\alpha_1 - \gamma_1^2}, \tag{3.1.157}$$

and, therefore, by (3.1.155) with $n = 2$, and (3.1.156),

$$(\boldsymbol{A}^{-1})_{ii} > \frac{\sum_{k\neq i} \sum_{\ell\neq i} a_{k\ell} a_{ki} a_{\ell i}}{a_{ii} \sum_{k\neq i} \sum_{\ell\neq i} a_{k\ell} a_{ki} a_{\ell i} - \left(\sum_{k\neq i} a_{ki}^2\right)^2}. \tag{3.1.158}$$

In the case of $(n+1)$-point Gauss–Radau formulae, we can proceed in the same manner, using Remark (c) to Theoree 3.2 and an analogous remark relating to (3.1.21). When $n=1$, one gets from (3.1.14) and the fact that $\beta_j = \gamma_j^2$,

$$\boldsymbol{J}_2^{R,a}(\mathrm{d}\rho_N) = \begin{bmatrix} \alpha_0 & \gamma_1 \\ \gamma_1 & \alpha_1^R \end{bmatrix}, \quad \alpha_1^R = a + \frac{\gamma_1^2}{\alpha_0 - a},$$

where $\alpha_0 = a_{ii}$ and $\gamma_1 = s_i$ from (3.1.156). Replacing a by b in α_1^R gives $\boldsymbol{J}_2^{R,b}(\mathrm{d}\rho_N)$. From (3.1.157), where α_1 is replaced by α_1^R, and recalling that the left-handed (right-handed) Gauss–Radau formula yields an upper (lower) bound, one finds by a simple computation that

$$\frac{a_{ii} - b + s_i^2/b}{a_{ii}^2 - a_{ii}b + s_i^2} < (\boldsymbol{A}^{-1})_{ii} < \frac{a_{ii} - a + s_i^2/a}{a_{ii}^2 - a_{ii}a + s_i^2}. \tag{3.1.159}$$

We finally note from Theorem 3.7 and the first inequality in (3.1.154) that the $(n+2)$-point Gauss–Lobatto formula provides another upper bound. Taking $n=0$ in (3.1.27), we have

$$\boldsymbol{J}_2^{L}(\mathrm{d}\rho_N) = \begin{bmatrix} \alpha_0 & \gamma_1^L \\ \gamma_1^L & \alpha_1^L \end{bmatrix},$$

where by (3.1.28) the quantities α_1^L and γ_1^L satisfy the 2×2 system

$$\begin{bmatrix} a-\alpha_0 & 1 \\ b-\alpha_0 & 1 \end{bmatrix} \begin{bmatrix} \alpha_1^L \\ (\gamma_1^L)^2 \end{bmatrix} = \begin{bmatrix} a(a-\alpha_0) \\ b(b-\alpha_0) \end{bmatrix}, \quad \alpha_0 = a_{ii}.$$

Solving for α_1^L, $(\gamma_1^L)^2$ and substituting the result in (3.1.157) in place of α_1 and γ_1^2 yields

$$(\boldsymbol{A}^{-1})_{ii} < \frac{a+b-a_{ii}}{ab}. \tag{3.1.160}$$

The bounds in (3.1.160) and (3.1.159) look simpler than those in (3.1.158), but unlike (3.1.158), they require information about the spectrum of $\boldsymbol{A}$.

3.2 Least squares approximation

Since (discrete) orthogonal polynomials arose in Chebyshev's (1859) work on polynomial fitting of discrete data by means of the least squares principle, it seems appropriate to begin with a brief account of the problem and its solution. This will be followed by various extensions.

3.2.1 *Classical least squares approximation*

Given N discrete data points (t_k, f_k), $k = 1, 2, \ldots, N$, and corresponding positive weights w_k, the problem is to determine a polynomial $\hat{p}_n \in \mathbb{P}_n$ of degree $n < N$ such that

$$\sum_{k=1}^{N} w_k[\hat{p}_n(t_k) - f_k]^2 \leq \sum_{k=1}^{N} w_k[p(t_k) - f_k]^2 \quad \text{for all } p \in \mathbb{P}_n. \tag{3.2.1}$$

It is natural to associate with this problem the discrete measure $\mathrm{d}\lambda_N$ supported on the points $t_1, t_2, \ldots, t_N$ and having jumps w_k at t_k, and the inner product and norm (cf. (1.1.12))

$$(u, v)_{\mathrm{d}\lambda_N} = \sum_{k=1}^{N} w_k u(t_k) v(t_k), \quad \|u\|_{\mathrm{d}\lambda_N} = \sqrt{(u, u)_{\mathrm{d}\lambda_N}}. \tag{3.2.2}$$

Then, (3.2.1) can be given the form

$$\|\hat{p}_n - f\|^2_{\mathrm{d}\lambda_N} \leq \|p - f\|^2_{\mathrm{d}\lambda_N} \quad \text{for all } p \in \mathbb{P}_n. \tag{3.2.3}$$

Thus, we want to minimize the squared error E_n^2 on the right of (3.2.3) over all polynomials $p \in \mathbb{P}_n$.

The solution is immediate if we express p in terms of the discrete orthogonal polynomials $\pi_k(\,\cdot\,) = \pi_k(\,\cdot\,; \mathrm{d}\lambda_N)$ (not necessarily monic) as

$$p(t) = \sum_{i=0}^{n} c_i \pi_i(t), \quad n < N, \tag{3.2.4}$$

and write, using the orthogonality of the π_k,

$$\begin{aligned} E_n^2 &= \left(\sum_{i=0}^{n} c_i \pi_i - f, \sum_{j=0}^{n} c_j \pi_j - f \right) = \sum_{i,j=0}^{n} c_i c_j (\pi_i, \pi_j) - 2 \sum_{i=0}^{n} c_i (f, \pi_i) + \|f\|^2 \\ &= \sum_{i=0}^{n} \left(\|\pi_i\| c_i - \frac{(f, \pi_i)}{\|\pi_i\|} \right)^2 + \|f\|^2 - \sum_{i=0}^{n} \frac{(f, \pi_i)^2}{\|\pi_i\|^2}. \end{aligned} \tag{3.2.5}$$

(Here and in the following, all inner products and norms are relative to the measure $\mathrm{d}\lambda_N$.) The minimum is clearly attained for $c_i = \hat{c}_i(f)$, where

$$\hat{c}_i(f) = \frac{(f, \pi_i)}{\|\pi_i\|^2}, \quad i = 0, 1, \ldots, n. \tag{3.2.6}$$

These are nothing but the "Fourier coefficients" of f relative to the orthogonal system $\pi_0, \pi_1, \ldots, \pi_{N-1}$. Moreover, the least squares error $\hat{E}_n$ becomes

$$\hat{E}_n = \left(\|f\|^2 - \sum_{i=0}^{n} |\hat{c}_i(f)|^2 \|\pi_i\|^2 \right)^{1/2}, \tag{3.2.7}$$

as follows from (3.2.5) with $c_i = \hat{c}_i(f)$ and (3.2.6). Since the error is nonnegative, we have that

$$\sum_{i=0}^{n} |\hat{c}_i(f)|^2 \|\pi_i\|^2 \le \|f\|^2, \quad n < N. \tag{3.2.8}$$

In the limit case $n = N-1$, the error $\hat{E}_n$ can be driven down to zero by taking for $\hat{p}_n$ the polynomial of degree $\le N-1$ interpolating f at the points $t_1, t_2, \ldots, t_N$. Therefore,

$$\sum_{i=0}^{N-1} |\hat{c}_i(f)|^2 \|\pi_i\|^2 = \|f\|^2, \tag{3.2.9}$$

which may be called the (discrete) *completeness relation*.

While expression (3.2.7) for the error is mathematically elegant, it is not recommended for computation. The reason is that the quantity under the radical sign, when evaluated in machine arithmetic, is in the best of circumstances of the order of the machine precision ε, hence $\hat{E}_n$ of the order $\sqrt{\varepsilon}$, which may be unrealistically large. In contrast, if the error is evaluated from its definition

$$\hat{E}_n = \left(\sum_{k=1}^{N} w_k [\hat{p}_n(t_k) - f_k]^2 \right)^{1/2},$$

then for errors near machine precision, the radicand is $O(\varepsilon^2)$; hence, $\hat{E}_n = O(\varepsilon)$.

Numerical problems may also arise in computing the Fourier coefficients $\hat{c}_i(f)$ in (3.2.6), as the evaluation of the inner product in the numerator of (3.2.6) may be subject to cancellation. As i becomes large, the problem typically worsens, but can be mitigated somewhat by replacing (3.2.6) with

$$\hat{c}_i(f) = \frac{1}{\|\pi_i\|^2} \left(f - \sum_{j=0}^{i-1} \hat{c}_j(f)\pi_j, \pi_i \right), \quad i = 0, 1, \ldots, n, \tag{3.2.10}$$

which is mathematically, though not numerically, equivalent to (3.2.6). The empty sum (when $i = 0$), of course, is meant to be zero.

From the $N \times (n+1)$ array of orthogonal polynomials π_i, $i = 0, 1, \ldots, n$, evaluated at the points t_k, the corresponding array of least squares polynomials $\hat{p}_i$, along with the $(n+1)$-vector of Fourier coefficients $\hat{c}_i$ can be generated as shown in Algorithm 3.4. The values f_k of the given data are input through the N-vector f.

Algorithm 3.4 (Polynomial least squares approximation)

Initialization:

$$\hat{p}_{-1} = 0, \quad e_{-1} = f.$$

Continuation: for $i = 0, 1, \ldots, n$ do

$$\hat{c}_i = \frac{1}{\|\pi_i\|^2}(e_{i-1}, \pi_i),$$
$$\hat{p}_i = \hat{p}_{i-1} + \hat{c}_i \pi_i,$$
$$e_i = e_{i-1} - \hat{c}_i \pi_i \quad (\text{if } i < n).$$

Algorithm 3.4 is implemented in the OPQ routine `least_squares.m`.

Example 3.48 Least squares approximation on equally spaced points.

We apply Algorithm 3.4 in the case of N equally spaced points $t_k = -1 + 2(k-1)/(N-1)$ on $[-1, 1]$ and equal weights $w_k = 2/N$. The orthogonal polynomials π_i are then the appropriately scaled discrete Chebyshev polynomials of Example 1.15. The computations are done in the OPQ routine `Example3_48.m`, the core of which is shown below.

```
k=(1:N)'; E2=zeros(N,1); Einf=zeros(N,1);
xw(k,1)=-1+2*(k-1)/(N-1); xw(:,2)=2/N; d=ones(1,N);
ab=r_hahn(N-1);
ab(:,1)=-1+2*ab(:,1)/(N-1);
ab(:,2)=(2/(N-1))^2*ab(:,2); ab(1,2)=2;
%
% The (Nx1)-vector f is assumed to contain the values
% of f at xw(:,1).
%
[phat,c]=least_squares(N-1,f,xw,ab,d);
t=linspace(-1,1); p=zeros(100,N);
%
% The (100x1)-vector ft is assumed to contain the
% values of f at t.
%
for n=1:N
   E2(n)=sqrt(sum(xw(:,2).*((phat(:,n)-f).^2)));
   p(:,n)=clenshaw(n-1,t,1,0,ab,c);
   Einf(n)=max(abs(p(:,n)-ft));
end
```

Although, in practice, the algorithm is most useful for experimental data, we apply it here to mathematically defined functions f of various degrees of smoothness, specifically to $f(t) = \mathrm{e}^{-t}$, $f(t) = \ln(2+t)$, $f(t) = \sqrt{1+t}$, and $f(t) = |t|$. The errors achieved for $N = 10$ and selected values of n are shown in Table 3.13, not only the least squares errors $\hat{E}_n$, but also the maximum errors E_n^∞ over 100 equally spaced points on $[-1, 1]$. Note that $\hat{E}_{N-1}$ is essentially zero in all cases, reflecting the interpolation property of $\hat{p}_{N-1}$. Otherwise, the two errors $\hat{E}_n$ and E_n^∞ are of comparable magnitude, their rate of convergence decreasing as one proceeds from left to right, that is, from functions with higher to functions with lower regularity.

An (absolutely continuous) measure $\mathrm{d}\lambda$ given on some interval $[a, b]$ generates interesting classes of least squares approximants. Indeed, we may take for the

Table 3.13 *Least squares and maximum errors for Example 3.48.*

	$f(t)=\mathrm{e}^{-t}$		$f(t)=\ln(2+t)$		$f(t)=\sqrt{1+t}$		$f(t)=\lvert t\rvert$	
n	$\hat{E}_n$	E_n^∞	$\hat{E}_n$	E_n^∞	$\hat{E}_n$	E_n^∞	$\hat{E}_n$	E_n^∞
0	1.05(+00)	1.50(+00)	4.88(–01)	6.37(–01)	5.86(–01)	9.10(–01)	4.44(–01)	5.46(–01)
3	6.16(–03)	6.61(–03)	2.96(–03)	3.49(–03)	4.83(–02)	1.01(–01)	1.02(–01)	1.98(–01)
6	2.45(–06)	6.25(–06)	2.07(–05)	7.06(–05)	4.73(–03)	7.99(–02)	1.86(–02)	8.51(–02)
9	6.08(–16)	3.84(–09)	1.74(–16)	3.44(–06)	1.56(–16)	6.79(–02)	1.35(–16)	6.50(–02)

points t_k and weights w_k either the nodes and weights

$$t_k = \tau_k^G, \quad w_k = \lambda_k^G, \quad k = 1, 2, \ldots, N, \tag{3.2.11}$$

of the N-point Gauss quadrature rule for the measure $\mathrm{d}\lambda$ (cf. (3.1.1)), or else, if $[a, b]$ is finite, the nodes and weights

$$t_k = \tau_k^L, \quad w_k = \lambda_k^L, \quad k = 1, 2, \ldots, N, \tag{3.2.12}$$

of the N-point Gauss–Lobatto quadrature rule (cf. (3.1.26)) (in which case $t_1 = a$, $t_N = b$). In either case, by Theorems 1.22 and 1.23, the discrete orthogonal polynomials are $\pi_k(\,\cdot\,; \mathrm{d}\lambda_N) = \pi_k(\,\cdot\,; \mathrm{d}\lambda)$, $k = 0, 1, \ldots, N-1$, that is, the first N orthogonal polynomials belonging to $\mathrm{d}\lambda$. We illustrate this for the Chebyshev measure $\mathrm{d}\lambda(t) = (1-t^2)^{-1/2}\mathrm{d}t$ on $[-1, 1]$.

Example 3.49 Least squares approximants with Gauss points and weights.

From Example 1.49 we have

$$t_k = \cos\frac{2k-1}{2N}\,\pi, \quad w_k = \frac{\pi}{N}\,, \quad k = 1, 2, \ldots, N,$$

and we may take for the π_i the Chebyshev polynomials T_i of the first kind. We recall from the Commentary to Table 1.1 and the fact that the N-point Gauss rule is exact for polynomials of degree $\leq 2N-1$ that

$$\|T_0\|^2 = \pi, \quad \|T_i\|^2 = \tfrac{1}{2}\,\pi, \quad i = 1, 2, \ldots, N-1.$$

The Fourier coefficients (3.2.6), therefore, become

$$\hat{c}_i(f) = \frac{2}{N}\sum_{k=1}^{N} f(t_k)T_i(t_k), \quad i = 0, 1, \ldots, N-1, \tag{3.2.13}$$

except for a factor $\frac{1}{2}$ when $i = 0$. The least squares approximant, thus, is

$$\hat{p}_n(t) = \tfrac{1}{2}\hat{c}_0(f) + \sum_{i=1}^{n} \hat{c}_i(f)T_i(t), \quad n < N,$$

with $\hat{c}_i(f)$ as defined in (3.2.13). The approximant can be evaluated by Clenshaw's algorithm; see Algorithm 2.3. The Fourier coefficients $\hat{c}_i(f)$ in (3.2.13) are evaluated by the `OPQ` routine `fourier_gauss.m`.

Example 3.50 Least squares approximants with Gauss–Lobatto points and weights.

Here, we have, from Example 1.50 (where n is replaced by $N-2$),

$$t_k = \cos\frac{N-k}{N-1}\,\pi, \quad k = 1, 2, \ldots, N,$$

and

$$w_1 = w_N = \frac{\pi}{2(N-1)}\,, \quad w_k = \frac{\pi}{N-1}\,, \quad k = 2, 3, \ldots, N-1.$$

By Theorem 1.23 (with n replaced by $N-2$), we may take again $\pi_i = T_i$ and proceed as in Example 3.49, the only difference being that now $\|T_{N-1}\|^2 = \pi$ (not $\frac{1}{2}\,\pi$) because of the extra term on the right of (1.2.5). Therefore,

$$\hat{c}_i(f) = \frac{2}{N-1}\,{\sum_{k=1}^{N}}'' f(t_k)T_i(t_k), \quad i = 0, 1, \ldots, N-1, \tag{3.2.14}$$

except that a factor $\frac{1}{2}$ is to be applied when $i = 0$ and $i = N-1$. The double prime on the summation sign indicates that the first and last terms in the sum are to be multiplied by $\frac{1}{2}$. Therefore,

$$\hat{p}_n(t) = \tfrac{1}{2}\hat{c}_0(f) + \chi_n \sum_{k=1}^{n} \hat{c}_i(f)T_i(t), \quad n < N,$$

where $\chi_{N-1} = \frac{1}{2}$ and $\chi_n = 1$ for $1 \le n < N-1$. This again can be evaluated by Clenshaw's Algorithm 2.3. The Fourier coefficients $\hat{c}_i(f)$ in (3.2.14) are evaluated by the `OPQ` routine `fourier_lobatto.m`.

The two approximants in Examples 3.49 and 3.50 give virtually identical answers when applied with $N = 10$ to the functions of Example 3.48, and answers very similar, though generally slightly better for the errors E_n^∞, to those in Table 3.13. See the routine `Example3_49.m`.

3.2.2 *Constrained least squares approximation*

It is sometimes desirable in least squares approximation to match a certain number of data points exactly, that is, to impose the constraints

$$p(s_j) = f_j, \quad j = 1, 2, \ldots, m; \quad m \le n, \tag{3.2.15}$$

where $\{s_1, s_2, \ldots, s_m\}$ may or may not be a subset of the points $\{t_1, t_2, \ldots, t_N\}$. We will denote by ν, $0 \le \nu \le m$, the number of s_j that are equal to one of the t_k. Let $p_m(f; \cdot)$ be the polynomial of degree $\le m-1$ interpolating f at the points s_j. We write

$$p(t) = p_m(f; t) + \sigma_m(t)q(t), \quad q \in \mathbb{P}_{n-m}, \tag{3.2.16}$$

where $\sigma_m(t) = \prod_{j=1}^{m}(t - s_j)$ and q is a polynomial of degree $n-m$ that can be freely varied. With notation as in §3.2.1, we then have

$$E_n^2 = \| f - p \|^2_{\mathrm{d}\lambda_N} = \| f - p_m(f;\,\cdot\,) - \sigma_m q \|^2_{\mathrm{d}\lambda_N}.$$

Here, the function to be minimized vanishes trivially at the points s_j, so that the discrete measure $\mathrm{d}\lambda_N$ may be replaced by $\mathrm{d}\lambda^*_{N-\nu}$ whose support is $\operatorname{supp}\mathrm{d}\lambda_N$ with ν of the s_j (those equal to some t_k) deleted, and whose jumps at the surviving support points are the original jumps of $\mathrm{d}\lambda_N$. Therefore,

$$E_n^2 = \| f - p_m(f;\,\cdot\,) - \sigma_m q \|^2_{\mathrm{d}\lambda^*_{N-\nu}} = \int_{\mathbb{R}} \left[\frac{f(t) - p_m(f;t)}{\sigma_m(t)} - q(t) \right]^2 \sigma_m^2(t) \mathrm{d}\lambda^*_{N-\nu},$$

and we are led to the unconstrained least squares problem

$$\text{minimize}: \quad \| f^* - q \|_{\mathrm{d}\lambda^*_N}, \quad q \in \mathbb{P}_{n-m}, \tag{3.2.17}$$

for a new function f^* and a new measure $\mathrm{d}\lambda^*_N$ given by

$$f^*(t) = \frac{f(t) - p_m(f;t)}{\sigma_m(t)}, \quad \mathrm{d}\lambda^*_N(t) = \sigma_m^2(t) \mathrm{d}\lambda^*_{N-\nu}(t). \tag{3.2.18}$$

If $\hat{q}_{n-m}$ is the solution of this problem, then

$$\hat{p}_n(t) = p_m(f;t) + \sigma_m(t) \hat{q}_{n-m}(t)$$

solves the constrained least squares problem.

The (discrete) orthogonal polynomials belonging to $\mathrm{d}\lambda^*_N$ can be generated by m successive applications of the `OPQ` routine `chri7.m` (cf. the end of §2.4.3), or else, by the Stieltjes procedure `stieltjes.m` (or Lanczos procedure `lanczos.m`); cf. §2.2.3.

As far as computing the function f^* is concerned, it is well known from the theory of polynomial interpolation that f^* can be written in terms of a divided difference of order m as

$$f^*(t) = [s_1, s_2, \ldots, s_m, t\,]f, \quad t \in \operatorname{supp}\mathrm{d}\lambda^*_{N-\nu}. \tag{3.2.19}$$

This can be computed either by the explicit formula

$$f^*(t) = \sum_{j=1}^{m} \frac{f(s_j)}{(s_j - t) \prod_{i \neq j} (s_j - s_i)} + \frac{f(t)}{\prod_j (t - s_j)}, \tag{3.2.20}$$

or generated "in place" by the following algorithm, written as a Matlab script,

```
for i=1:m+1, d(i)=f(i); end
for k=1:m
   for i=1:m-k+1
     d(i)=(d(i+1)-d(i))/(s(i+k)-s(i));
   end
end
```

At the beginning of the algorithm, the $(m+1)$-vector d contains the values of f at the points $s_1, s_2, \ldots, s_m, s_{m+1}$, where s_{m+1} is one of the support points of $\mathrm{d}\lambda^*_{N-\nu}$. After completion of the algorithm, d contains the divided differences $[s_i, s_{i+1}, \ldots, s_m, s_{m+1}]f$, $i = 1, 2, \ldots, m+1$. In particular, $d(1) = f^*(s_{m+1})$.

Example 3.51 The Bessel function J_0 on $[0, j_{0,3}]$.

We approximate the Bessel function J_0 of order zero on the interval from 0 to the third positive zero $j_{0,3}$ of J_0 and impose the constraint that the approximant vanish exactly at the first three zeros of J_0.

Here, $s_1 = j_{0,1}$, $s_2 = j_{0,2}$, $s_3 = j_{0,3}$ are the first three zeros of J_0, and the interpolation polynomial $p_3(J_0; \cdot)$ is identically zero, since we are interpolating at the zeros of J_0. Furthermore, by (3.2.20),

$$f^*(t) = \frac{J_0(t)}{\sigma_3(t)}, \quad \sigma_3(t) = (t - j_{0,1})(t - j_{0,2})(t - j_{0,3}).$$

The following routine, extracted from the `OPQ` routine `Example3_51.m`, calculates the constrained least squares polynomial $\hat{p}_n(t)$ of degree n at a given scalar- or vector-valued t, using N equally spaced points t_k on $[0, j_{0,3}]$ (end points included) and equal weights $w_k = 1/N$, $k = 1, 2, \ldots, N$. Since s_3 coincides with t_N, the measure $\mathrm{d}\lambda^*_N$ in (3.2.17) is $\mathrm{d}\lambda^*_N = \sigma_3^2(t)\mathrm{d}\lambda^*_{N-1}$.

```
s=[2.4048255577 5.5200781103 8.6537279129];
t1=linspace(0,s(3),N)';
N=N-1; m=3;
xw=zeros(N,2); d=ones(1,N);
t0=t1(1:N); f=bessel(0,t0);
xw=[t0,((t0-s(1)).*(t0-s(2)).*(t0-s(3))).^2/N];
ab=r_hahn(N-1);
ab(:,1)=t0(N)*ab(:,1)/(N-1); ab(:,2)=(t0(N)/(N-1))^2*ab(:,2);
ab(1,2)=1;
ab1=ab; ab=chri7(N-1,ab1,s(1));
ab1=ab; ab=chri7(N-2,ab1,s(2));
ab1=ab; ab=chri7(N-3,ab1,s(3));
f0=f./((t0-s(1)).*(t0-s(2)).*(t0-s(3)));
[qhat,c]=least_squares(n-m,f0,xw,ab,d);
x=linspace(0,s(3))'; p=zeros(100,n-m+1);
q=clenshaw(n-m,x,1,0,ab,c);
p(:,n-m+1)=(t-s(1)).*(t-s(2)).*(t-s(3)).*q;
```

When run with $N = 51$ and n=3:5:18, the routine produces least squares errors $\hat{E}_n$ and maximum errors E_n^∞ (over 100 equally spaced points on $[0, j_{0,3}]$) shown in Table 3.14. The approximants for $n = 3, 4$, and 5 are depicted in Fig. 3.3 (produced by the routine `Figure3_3.m`), where the solid curve represents the exact function, and the dashdotted, dashed, and dotted curves the constrained least squares approximants for $n = 3, 4$, and 5, respectively.

Table 3.14 *Least squares and maximum errors for Example 3.51.*

n	$\hat{E}_n$	E_n^∞
3	1.607(–01)	4.198(–01)
8	6.528(–04)	1.614(–03)
13	6.733(–08)	2.182(–07)
18	3.414(–12)	2.110(–11)

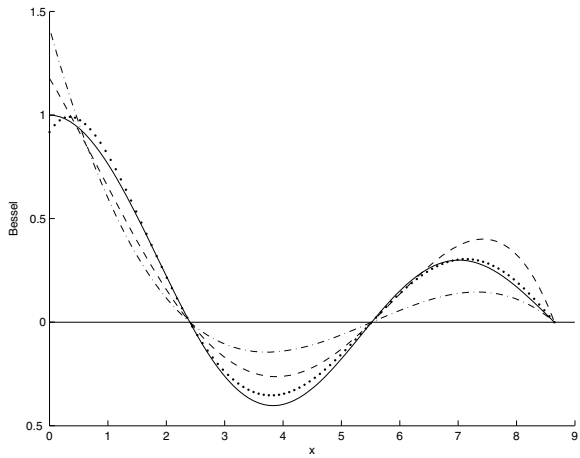

FIG. 3.3. Constrained least squares approximants to the Bessel function.

It is, in principle, possible to handle derivative constraints as well. The polynomial $p_m(f;\cdot)$ in (3.2.16) then must be the appropriate Hermite interpolation polynomial and the factor $t - s_j$ in $\sigma_m(t)$ has to be endowed with the appropriate multiplicity. Computing the divided difference in (3.2.19), which now has multiple points, may be cumbersome in general, but is relatively straightforward in special cases.

Example 3.52 The Bessel function J_0 on $[0, j_{0,3}]$, revisited.

The spurious behavior of the approximants near $t = 0$, exhibited in Fig. 3.3, can be eliminated, and the overall quality of the approximation enhanced, if we add the two constraints

$$p(0) = 1, \quad p'(0) = 0,$$

to the three already imposed in Example 3.51. Then $m = 5$, since to the three points s_1, s_2, s_3 a double point is added at the origin. The Hermite interpolation polynomial is found to be

$$p_5(J_0;t) = 1 - \frac{1}{s_1^2}\,t^2 + \frac{1}{s_1^2 s_2^2}\,(s_1+s_2)t^2(t-s_1) \\ -\frac{1}{s_1^2 s_2^2 s_3^2}\,(s_1 s_2 + s_1 s_3 + s_2 s_3)t^2(t-s_1)(t-s_2),$$

and the polynomial σ_5 in (3.2.16) becomes

$$\sigma_5(t) = t^2(t-s_1)(t-s_2)(t-s_3).$$

An elementary computation will show that

$$f^*(t) := [0,0,s_1,s_2,s_3,t\,]J_0 = \frac{J_0(t)}{\sigma_5(t)} + \frac{1+(\frac{1}{s_1}+\frac{1}{s_2}+\frac{1}{s_3})t}{s_1 s_2 s_3 t^2}\,.$$

The routine displayed in Example 3.51 and the routine `Figure3_3.m` require only minor modifications (two additional applications of `chri7.m` with

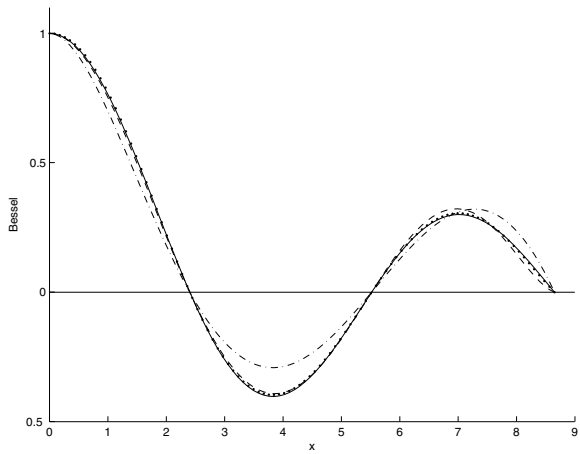

FIG. 3.4. Derivative-constrained least squares approximants to the Bessel function.

zero shifts, and changing the function `f0` and the polynomial `p`; see the routines `Example3_52.m` and `Figure3_4.m`). Yet, as is shown in Fig. 3.4, the approximants with $n = 5, 6$, and 7 are markedly improved compared with the corresponding approximants in Fig. 3.3.

3.2.3 *Least squares approximation in Sobolev spaces*

An extension of the classical least squares problem of §3.2.1, which attempts to simultaneously approximate function and derivative values, can be formulated as follows:

$$\text{minimize}: \quad \sum_{\sigma=0}^{s}\sum_{k=1}^{N} w_k^{(\sigma)}[p^{(\sigma)}(t_k) - f_k^{(\sigma)}]^2, \quad p \in \mathbb{P}_n, \tag{3.2.21}$$

where the minimum is taken over all polynomials p of degree $\leq n$. Here, $f_k^{(\sigma)}$, $\sigma = 0, 1, \ldots, s$, $s \geq 1$, are function and derivative values of f at t_k, and $w_k^{(\sigma)}$ are positive weights often chosen in terms of *one* set of positive weights w_k by defining

$$w_k^{(\sigma)} = \gamma_\sigma w_k, \quad \gamma_\sigma > 0, \quad k = 1, 2, \ldots, N. \tag{3.2.22}$$

The appropriate inner product and norm are those of Sobolev type,

$$(u, v)_S = \sum_{\sigma=0}^{s} \sum_{k=1}^{N} w_k^{(\sigma)} u^{(\sigma)}(t_k) v^{(\sigma)}(t_k), \quad \|u\|_S = \sqrt{(u, u)_S}. \tag{3.2.23}$$

The solution of (3.2.21) is entirely analogous to the classical solution process, except that inner products and norms are to be replaced throughout by the Sobolev inner products and Sobolev norms of (3.2.23) and the orthogonal polynomials are the Sobolev orthogonal polynomials (cf. §1.7). Thus, in particular, we can write the solution $\hat{p}_n$ in the form

$$\hat{p}_n(t) = \sum_{i=0}^{n} \hat{c}_i \pi_i(t), \quad \hat{c}_i = \frac{(f, \pi_i)_S}{\|\pi_i\|_S^2}, \tag{3.2.24}$$

where the data f now consist of the values and the first s derivatives of the given function at the points t_k, and π_i are the Sobolev orthogonal polynomials belonging to the inner product (3.2.23). Likewise, Algorithm 3.4 has its exact analog in the present context, producing the least squares approximants and their first s derivatives at the points t_k, along with the Fourier coefficients.

Algorithm 3.5 (Polynomial least squares approximation in Sobolev spaces)
Initialization:

$$\hat{p}_{-1} = 0, \quad e_{-1} = f.$$

Continuation: for $i = 0, 1, \ldots, n$ do

$$\begin{aligned} \hat{c}_i &= \frac{1}{\|\pi_i\|_S^2}(e_{i-1}, \pi_i)_S, \\ \hat{p}_i &= \hat{p}_{i-1} + \hat{c}_i \pi_i, \\ e_i &= e_{i-1} - \hat{c}_i \pi_i \quad (\text{if } i < n). \end{aligned}$$

Algorithm 3.5 is implemented in the `OPQ` routine `least_squares_sob.m`.

This kind of approximation is attractive when derivatives are easy to come by.

Example 3.53 Complementary error function.
Consider the function

$$f(t) = \mathrm{e}^{t^2} \operatorname{erfc} t = \frac{2}{\sqrt{\pi}} \mathrm{e}^{t^2} \int_t^\infty \mathrm{e}^{-u^2} \, \mathrm{d}u$$

on the interval $[0, 2]$. Its derivatives are easily generated; the first two are

$$f'(t) = 2tf(t) - \frac{2}{\sqrt{\pi}}, \quad f''(t) = 2(1 + 2t^2)f(t) - \frac{4}{\sqrt{\pi}}\,t.$$

We apply the `OPQ` routine `least_squares_sob.m` with $s = 2$ using $N = 5$ equally spaced points t_k on $[0, 2]$ (end points included) and the same equal weights $w_k^{(\sigma)} = 1/N$ for $\sigma = 0, 1, 2$. In Table 3.15 (which is analogous to Table 3.13), we show in the top half selected results for the Sobolev least squares error $\hat{E}_n$ and the

Table 3.15 *Sobolev least squares errors vs ordinary least squares errors, and maximum errors, for Example 3.53.*

n	$\hat{E}_n$	$E_{n,0}^{\infty}$	$E_{n,1}^{\infty}$	$E_{n,2}^{\infty}$
0	1.153(+00)	4.759(–01)	1.128(+00)	2.000(+00)
2	7.356(–01)	8.812(–02)	2.860(–01)	1.411(+00)
4	1.196(–01)	1.810(–02)	5.434(–02)	1.960(–01)
9	2.178(–05)	4.710(–06)	3.011(–05)	3.159(–04)
14	3.653(–16)	1.130(–09)	1.111(–08)	1.966(–07)
0	2.674(–01)	4.759(–01)	1.128(+00)	2.000(+00)
2	2.245(–02)	3.865(–02)	3.612(–01)	1.590(+00)
4	1.053(–16)	3.516(–03)	5.160(–02)	4.956(–01)
9	1.053(–16)	5.409(–03)	8.124(–02)	7.959(–01)
14	1.053(–16)	5.478(–03)	8.226(–02)	8.057(–01)

maximum errors $E_{n,0}^{\infty}$, $E_{n,1}^{\infty}$, $E_{n,2}^{\infty}$ over 100 equally spaced points on $[0, 2]$ for the function and its first two derivatives. In the bottom half are shown the analogous results for ordinary least squares approximation ($s = 0$). Complete results can be had by running the routine `Example3_53.m`. Note that in the case of Sobolev least squares, the L_2 error $\hat{E}_{3N-1}$ is essentially zero, as it should be, given that the Hermite interpolation polynomial of degree $3N - 1$ interpolates the data exactly. In contrast, we have $\hat{E}_n = 0$ for $n \geq N - 1$ in the case of ordinary least squares. The table also shows rather convincingly, and as expected, that Sobolev least squares approximation approximates the derivatives decidedly better than ordinary least squares approximation, and even the function itself when n is sufficiently large.

3.3 Moment-preserving spline approximation

The moments of a function (or a distribution) often have physical meaning. When trying to approximate the function, it may be desirable to preserve the moments, that is, to choose the approximation in such a way that as many of its moments as possible are the same as those of the given function. Instances of this have appeared in the physics literature, for example in the approximation of the Maxwell velocity distribution by a linear combination of Dirac δ-functions

(Laframboise and Stauffer, 1969) or by a linear combination of Heaviside step functions (Calder and Laframboise, 1986). The solutions given in the cited references use classical methods—Prony's method in the former, and a reduction to a Hankel matrix eigenvalue problem in the latter reference. Both approaches are sensitive to rounding errors, and thus require high-precision calculations. It is possible, however, to exploit the close connection of these problems with Gaussian quadrature to arrive at more stable solution procedures that are applicable also in the case of more general approximation problems involving variable-knot polynomial spline functions. We begin in §3.3.1 with the physically important case of approximation on the positive real line and discuss the more difficult case of a compact interval in §3.3.2.

3.3.1 *Approximation on the positive real line*

3.3.1.1 *Approximation by step functions* We consider a function $f = f(t)$ defined on the positive real line $\mathbb{R}_+ = \{t : \ 0 \le t < \infty\}$ and wish to approximate it by a linear combination of Heaviside step functions,

$$s_n(t) = \sum_{\nu=1}^{n} a_\nu H(t_\nu - t), \quad t \in \mathbb{R}_+, \tag{3.3.1}$$

where H is defined by

$$H(u) = \begin{cases} 1 & \text{if } u \ge 0, \\ 0 & \text{if } u < 0. \end{cases} \tag{3.3.2}$$

The "knots" t_ν are assumed distinct and ordered increasingly, $0 < t_1 < t_2 < \cdots < t_n$, and $a_\nu \in \mathbb{R}$. We seek an approximation such that

$$\int_0^\infty s_n(t) t^j \, \mathrm{d}t = \mu_j, \quad j = 0, 1, \ldots, 2n-1, \tag{3.3.3}$$

where[6]

$$\mu_j = \int_0^\infty f(t) t^j \, \mathrm{d}t \tag{3.3.4}$$

are the moments of f. Note that all a_ν and t_ν in (3.3.1) are considered unknowns that can be freely chosen subject to the ordering of t_ν. Since there are $2n$ of them, it seems plausible that $2n$ conditions, such as those in (3.3.3), can be imposed to uniquely determine them. That this, under suitable conditions, is indeed the case is the content of the following theorem, which also tells us how s_n, if it exists, can be constructed.

Theorem 3.54 *For fixed $n \in \mathbb{N}$, let f satisfy the following conditions:*

[6] In applications to physics, the moments may be defined with respect to a surface differential $\mathrm{d}V$. Depending on the geometry of the problem, the differential, up to unimportant numerical factors, is $\mathrm{d}V = \mathrm{d}t$ for rectilinear geometry, $\mathrm{d}V = t\,\mathrm{d}t$ for cylindrical geometry, and $\mathrm{d}V = t^2\,\mathrm{d}t$ for spherical geometry. Our discussion is for $\mathrm{d}V = \mathrm{d}t$, but can easily be adapted to the other two cases.

(i) $f \in C^1(\mathbb{R}_+)$;
(ii) *the first* $2n$ *moments (3.3.4) of* f *exist;*
(iii) $f(t) = o(t^{-2n})$ *as* $t \to \infty$.

Then, the approximation problem (3.3.1)–(3.3.3) has a unique solution if and only if the measure

$$\mathrm{d}\lambda(t) = -tf'(t)\,\mathrm{d}t \quad \textit{on } \mathbb{R}_+ \tag{3.3.5}$$

admits a Gaussian quadrature formula (cf. (3.1.1))

$$\int_0^\infty g(t)\,\mathrm{d}\lambda(t) = \sum_{\nu=1}^{n} \lambda_\nu^G g(\tau_\nu^G) \quad \textit{for all } g \in \mathbb{P}_{2n-1}, \tag{3.3.6}$$

satisfying $0 < \tau_1^G < \tau_2^G < \cdots < \tau_n^G$. *If that is the case, the knots* t_ν *and coefficients* a_ν *in (3.3.1) are given by*

$$t_\nu = \tau_\nu^G, \quad a_\nu = \frac{\lambda_\nu^G}{\tau_\nu^G}, \quad \nu = 1, 2, \ldots, n. \tag{3.3.7}$$

Proof We first use integration by parts to express the moments of f in terms of those of the measure $\mathrm{d}\lambda$ in (3.3.5),

$$\mu_j = \frac{1}{j+1} \int_0^\infty t^j\,\mathrm{d}\lambda(t), \quad j = 0, 1, \ldots, 2n-1. \tag{3.3.8}$$

Indeed, for any $T > 0$, there holds

$$\int_0^T f(t)t^j\,\mathrm{d}t = \frac{1}{j+1}\, t^{j+1} f(t)\Big|_0^T - \frac{1}{j+1} \int_0^T f'(t)t^{j+1}\,\mathrm{d}t.$$

As $T \to \infty$, the left-hand side tends to the moment μ_j by assumption (ii) and the first term on the right to zero by assumption (iii). Therefore, the second term on the right-hand side also has a finite limit as $T \to \infty$, which, in fact, is given by (3.3.8) by virtue of the definition of $\mathrm{d}\lambda$ in (3.3.5).

The moments of s_n, on the other hand, are easily computed to be

$$\int_0^\infty s_n(t)t^j\,\mathrm{d}t = \sum_{\nu=1}^{n} a_\nu \int_0^{t_\nu} t^j\,\mathrm{d}t = \frac{1}{j+1} \sum_{\nu=1}^{n} a_\nu t_\nu^{j+1}.$$

The moment-matching equations (3.3.3), thus, become

$$\sum_{\nu=1}^{n} (a_\nu t_\nu) t_\nu^j = \int_0^\infty t^j\,\mathrm{d}\lambda(t), \quad j = 0, 1, \ldots, 2n-1,$$

which are precisely the equations stating that $t_\nu = \tau_\nu^G$ and $a_\nu t_\nu = \lambda_\nu^G$ for $\nu = 1, 2, \ldots, n$. □

If the function f, in addition to satisfying the conditions (i)–(iii) of Theorem 3.54, is decreasing on $\mathbb{R}_+$, then the measure $\mathrm{d}\lambda$ of (3.3.5) is positive, and the Gauss formula (3.3.6) exists. The step function s_n satisfying (3.3.3), therefore, exists uniquely.

Example 3.55 The Maxwell distribution.

This is the case $f(t) = \mathrm{e}^{-t^2}$, for which $\mathrm{d}\lambda(t) = 2t^2\mathrm{e}^{-t^2}\,\mathrm{d}t$ on $\mathbb{R}_+$. The Gauss formula for $\mathrm{d}\lambda$ is readily obtained from the recurrence coefficients $\alpha_k(\mathrm{d}\lambda)$ and $\beta_k(\mathrm{d}\lambda)$, which, in turn, can be obtained from those of the half-range Hermite measure (Example 2.31) by two applications of Algorithm 2.5. The desired step function approximation is computed and plotted by the `OPQ` routine `Example3_55.m`, using the following script for calculating the knots t_ν and coefficients a_ν (stored in the array `ta`):

```
load -ascii abhrhermite;
ab0=abhrhermite(1:n+2,:);
ab1=chri1(n+1,ab0,0);
ab=chri1(n,ab1,0); ab(1,2)=sqrt(pi)/2;
ta=gauss(n,ab);
ta(:,2)=ta(:,2)./ta(:,1);
```

The file `abhrhermite` contains the first 100 recurrence coefficients of the half-range Hermite measure. The results for $n = 5$ are shown in Table 3.16 and depicted in Figure 3.5.

Table 3.16 *Step function approximation of the Maxwell distribution.*

ν	t_ν	a_ν
1	0.3384096	0.2504936
2	0.8266625	0.4613997
3	1.4328544	0.2418570
4	2.1454082	0.0332937
5	3.0141725	0.0006839

3.3.1.2 *Approximation by Dirac delta functions* The approximant now takes the form

$$d_n(t) = \sum_{\nu=1}^{n} a_\nu \delta(t - t_\nu), \quad t \in \mathbb{R}_+, \tag{3.3.9}$$

where $\delta(\,\cdot\,)$ is the Dirac delta function, and the moment-matching conditions as before are

$$\int_0^\infty d_n(t) t^j \,\mathrm{d}t = \mu_j, \quad j = 0, 1, \ldots, 2n-1. \tag{3.3.10}$$

In this case there is always a unique solution if f is positive on $\mathbb{R}_+$. The following theorem indeed is almost self-evident.

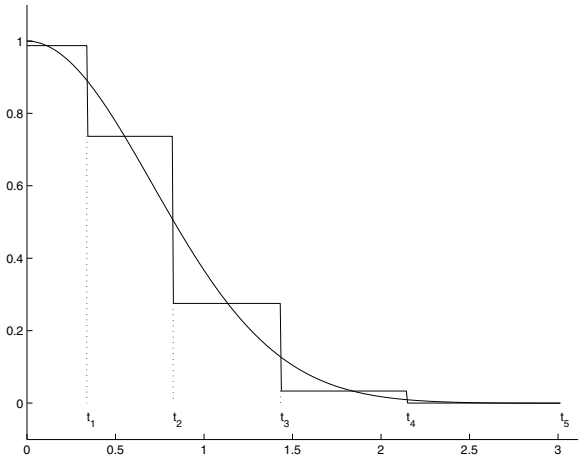

FIG. 3.5. Moment-preserving step function approximation to the Maxwell distribution.

Theorem 3.56 *Let $f \geq 0$ on $\mathbb{R}_+$ (and $f > 0$ on a set of positive measure), and assume that the first $2n$ moments μ_j, $j = 0, 1, \ldots, 2n-1$, of f exist. Then, the approximation problem (3.3.9)–(3.3.10) has a unique solution given by*

$$t_\nu = \tau_\nu^G, \quad a_\nu = \lambda_\nu^G, \quad \nu = 1, 2, \ldots, n, \tag{3.3.11}$$

where τ_ν^G, λ_ν^G are the nodes and weights of the n-point Gauss quadrature rule for the measure $\mathrm{d}\lambda(t) = f(t)\,\mathrm{d}t$.

3.3.1.3 *Approximation by spline functions* The theory developed in the previous subsections can be extended to spline functions of arbitrary degree m, the case $m = 0$ corresponding to step functions, and $m = -1$ (in a manner of speaking) to Dirac delta functions. Since we continue to consider approximation on the positive real line $\mathbb{R}_+$, and the approximants are to have finite moments, the splines cannot have a purely polynomial component and, hence, must vanish at infinity. Such splines, of degree $m \geq 0$ with n distinct positive knots t_ν, $\nu = 1, 2, \ldots, n$, can be written in the form

$$s_{n,m}(t) = \sum_{\nu=1}^{n} a_\nu (t_\nu - t)_+^m, \quad t \in \mathbb{R}_+, \tag{3.3.12}$$

where $u_+ = uH(u)$, with H the Heaviside step function (3.3.2), $0 < t_1 < t_2 < \cdots < t_n$, and $a_\nu \in \mathbb{R}$. We seek to determine $s_{n,m}$ such that

$$\int_0^\infty s_{n,m}(t) t^j \,\mathrm{d}t = \mu_j, \quad j = 0, 1, \ldots, 2n-1, \tag{3.3.13}$$

where μ_j are the moments (3.3.4) of the given function f.

Theorem 3.57 *For fixed $m, n \in \mathbb{N}$, let f satisfy the following conditions:*

(i) $f \in C^{m+1}(\mathbb{R}_+)$;

(ii) *the first $2n$ moments (3.3.4) of f exist;*

(iii) $f^{(\mu)}(t) = o(t^{-2n-\mu})$ *as* $t \to \infty$, $\mu = 0, 1, \ldots, m$.

Then, the approximation problem (3.3.12)–(3.3.13) has a unique solution if and only if the measure

$$\mathrm{d}\lambda^{[m]}(t) = \frac{(-1)^{m+1}}{m!}\, t^{m+1} f^{(m+1)}(t)\, \mathrm{d}t \quad \text{on } \mathbb{R}_+ \tag{3.3.14}$$

admits a Gaussian quadrature formula

$$\int_0^\infty g(t)\, \mathrm{d}\lambda^{[m]}(t) = \sum_{\nu=1}^{n} \lambda_\nu^G g(\tau_\nu^G) \quad \text{for all } g \in \mathbb{P}_{2n-1}, \tag{3.3.15}$$

satisfying $0 < \tau_1^G < \tau_2^G < \cdots < \tau_n^G$. If that is the case, the knots t_ν and coefficients a_ν in (3.3.12) are given by

$$t_\nu = \tau_\nu^G, \quad a_\nu = \frac{\lambda_\nu^G}{[\tau_\nu^G]^{m+1}}, \quad \nu = 1, 2, \ldots, n. \tag{3.3.16}$$

Proof Substituting (3.3.12) into (3.3.13) yields, since $t_\nu > 0$,

$$\sum_{\nu=1}^{n} a_\nu \int_0^{t_\nu} t^j (t_\nu - t)^m\, \mathrm{d}t = \int_0^\infty t^j f(t)\, \mathrm{d}t, \quad j = 0, 1, \ldots, 2n-1. \tag{3.3.17}$$

The left-hand side, through m integrations by parts, can be seen to equal

$$\begin{aligned} &\frac{m!}{(j+1)(j+2)\cdots(j+m)} \sum_{\nu=1}^{n} a_\nu \int_0^{t_\nu} t^{j+m}\, \mathrm{d}t \\ &\quad = \frac{m!}{(j+1)(j+2)\cdots(j+m+1)} \sum_{\nu=1}^{n} a_\nu t_\nu^{j+m+1}. \end{aligned} \tag{3.3.18}$$

The integral on the right in (3.3.17) is transformed similarly by $m+1$ integrations by parts. We carry out the first of them in detail to exhibit the reasonings involved. For any $T > 0$, we have

$$\int_0^T t^j f(t)\, \mathrm{d}t = \frac{1}{j+1}\, t^{j+1} f(t)\Big|_0^T - \frac{1}{j+1} \int_0^T t^{j+1} f'(t)\, \mathrm{d}t.$$

The integrated term clearly vanishes at $t = 0$ and tends to zero as $t = T \to \infty$ by assumption (iii) with $\mu = 0$. Since $j \le 2n - 1$ and the integral on the left

converges as $T \to \infty$ by assumption (ii), we infer the convergence of the integral on the right. Therefore,

$$\int_0^\infty t^j f(t)\,\mathrm{d}t = -\frac{1}{j+1}\int_0^\infty t^{j+1} f'(t)\,\mathrm{d}t.$$

Continuing in this manner, using assumption (iii) to show convergence to zero of the integrated term at the upper limit (its value at $t = 0$ always being zero) and the existence of $\int_0^\infty t^{j+\mu} f^{(\mu)}(t)\,\mathrm{d}t$ already established to infer the existence of $\int_0^\infty t^{j+\mu+1} f^{(\mu+1)}(t)\,\mathrm{d}t$, $\mu = 1, 2, \ldots, m$, we arrive at

$$\int_0^\infty t^j f(t)\,\mathrm{d}t = \frac{(-1)^{m+1}}{(j+1)(j+2)\cdots(j+m+1)}\int_0^\infty t^{j+m+1} f^{(m+1)}(t)\,\mathrm{d}t. \tag{3.3.19}$$

Comparing this with (3.3.18), we see that eqns (3.3.17), and hence eqns (3.3.13), are equivalent to

$$\sum_{\nu=1}^{n}(a_\nu t_\nu^{m+1})t_\nu^j = \int_0^\infty \left[\frac{(-1)^{m+1}}{m!}\,t^{m+1} f^{(m+1)}(t)\right] t^j\,\mathrm{d}t,$$
$$j = 0, 1, \ldots, 2n-1,$$

which are precisely the equations stating that $t_\nu = \tau_\nu^G$ are the nodes, and $a_\nu t_\nu^{m+1} = \lambda_\nu^G$ the weights, of the n-point Gauss formula for the measure $\mathrm{d}\lambda^{[m]}$ given in (3.3.14).

The nodes τ_ν^G, being the zeros of the orthogonal polynomial $\pi_n(\,\cdot\,;\mathrm{d}\lambda^{[m]})$ (if it exists), are uniquely determined, hence also the weights λ_ν^G. □

Theorem 3.57 reduces to Theorem 3.54 when $m = 0$. It becomes Theorem 3.56 if $m = -1$ and the factorial $m!$ in (3.3.14) is omitted. If f is *completely monotonic* on $\mathbb{R}_+$, that is, such that $(-1)^m f^{(m)}(t) > 0$ for all $t \in \mathbb{R}_+$ and all $m = 0, 1, 2, \ldots$, then the measure $\mathrm{d}\lambda^{[m]}$ in (3.3.14) is positive. Moreover, by (3.3.19), the first $2n$ moments of $\mathrm{d}\lambda^{[m]}$ exist, so that the Gauss formula (3.3.15) exists and has distinct positive nodes τ_ν^G and positive weights λ_ν^G. The latter implies $a_\nu > 0$ in (3.3.12) and thus the complete monotonicity of the spline approximant in the weak sense $(-1)^m s_{n,m}^{(m)}(t) \geq 0$.

Theorem 3.58 *Let*

$$\sigma_t^{[m]}(s) = s^{-(m+1)}(s-t)_+^m, \quad s > 0,\ t > 0. \tag{3.3.20}$$

Then, in the affirmative case of Theorem 3.57, there holds, for any $t > 0$,

$$f(t) - s_{n,m}(t) = R_n(\sigma_t^{[m]}), \tag{3.3.21}$$

where $R_n(\sigma)$ is the remainder term of the Gauss quadrature formula (3.3.15),

$$\int_0^\infty \sigma(s)\,\mathrm{d}\lambda^{[m]}(s) = \sum_{\nu=1}^{n}\lambda_\nu^G\sigma(\tau_\nu^G) + R_n(\sigma). \tag{3.3.22}$$

Proof For any $T > 0$, one has by Taylor's formula

$$f(t) = f(T) + f'(T)(t-T) + \cdots + \frac{1}{m!} f^{(m)}(T)(t-T)^m + \frac{1}{m!} \int_T^t (t-s)^m f^{(m+1)}(s)\, \mathrm{d}s. \tag{3.3.23}$$

Since by assumption (iii) of Theorem 3.57, $\lim_{T\to\infty} T^\mu f^{(\mu)}(T) = 0$ for $\mu = 0, 1, \ldots, m$, letting $T \to \infty$ in (3.3.23) gives

$$f(t) = \frac{(-1)^{m+1}}{m!} \int_t^\infty (s-t)^m f^{(m+1)}(s)\, \mathrm{d}s = \frac{(-1)^{m+1}}{m!} \int_0^\infty (s-t)_+^m f^{(m+1)}(s)\, \mathrm{d}s.$$

Therefore, by (3.3.20) and (3.3.14),

$$f(t) = \int_0^\infty \sigma_t^{[m]}(s)\, \mathrm{d}\lambda^{[m]}(s). \tag{3.3.24}$$

On the other hand, by (3.3.12) and (3.3.16),

$$s_{n,m}(t) = \sum_{\nu=1}^n \frac{\lambda_\nu^G}{[\tau_\nu^G]^{m+1}} (\tau_\nu^G - t)_+^m = \sum_{\nu=1}^n \lambda_\nu^G \sigma_t^{[m]}(\tau_\nu^G).$$

Subtracting this from (3.3.24) yields (3.3.21). □

To discuss convergence as $n \to \infty$ (for fixed m), we assume that f satisfies assumptions (i)–(iii) of Theorem 3.57 for all $n = 1, 2, 3, \ldots$. Then, according to Theorem 3.58, our approximation process converges pointwise (at t), as $n \to \infty$, if and only if the Gauss quadrature formula (3.3.22) converges when applied to the particular function $\sigma(s) = \sigma_t^{[m]}(s)$ in (3.3.20). Since $\sigma_t^{[m]}$ is uniformly bounded on $\mathbb{R}$, this is true, for example, if $\mathrm{d}\lambda^{[m]}$ is a positive measure and the moment problem for $\mathrm{d}\lambda^{[m]}$ on $\mathbb{R}$ (with $\mathrm{d}\lambda^{[m]}(s) = 0$ for $s < 0$) is determined (cf. Freud (1971, Chapter 3, Theorem 1.1)).

Example 3.59 Exponential distribution.

Here, $f(t) = \mathrm{e}^{-t}$ on $\mathbb{R}_+$, and the measure $\mathrm{d}\lambda^{[m]}$ in (3.3.14) becomes the generalized Laguerre measure

$$\mathrm{d}\lambda^{[m]}(t) = \frac{1}{m!} t^{m+1} \mathrm{e}^{-t}\, \mathrm{d}t \quad \text{on } \mathbb{R}_+.$$

The knots t_ν of the spline (3.3.12), therefore, are the zeros of the generalized Laguerre polynomial $L_n^{(\alpha)}$ with parameter $\alpha = m + 1$ (cf. Commentary to Table 1.1), and the coefficients a_ν are readily computed from (3.3.16) in terms of the corresponding Gaussian weights λ_ν^G. The `OPQ` routine `Example3_59.m` computes $\|s_{n,m} - f\|_\infty$ for selected values of m and n, where the ∞-norm is relative to a set of 100 equally spaced points on $[0, t_n]$. (For $t > t_n$, one clearly has $|s_{n,m}(t) -$

Table 3.17 *The errors* $\|s_{n,m} - f\|_\infty$ *in Example 3.59.*

n	$m = 1$	$m = 2$	$m = 3$
5	4.7619(–2)	1.7857(–2)	7.9365(–3)
10	1.5405(–2)	3.4965(–3)	9.9900(–4)
20	5.1584(–3)	9.5823(–4)	1.3567(–4)
40	1.1614(–3)	3.7782(–4)	3.9944(–5)
80	3.0111(–4)	8.7392(–5)	7.1035(–6)

$f(t)| = f(t)$.) Since the moment problem for the generalized Laguerre measure is determined (Freud, 1971, Chapter 2, Theorem 5.2), it follows from the remark made in the sentence preceding this example that $s_{n,m}(t) \to f(t)$ as $n \to \infty$ for any fixed m and $t > 0$. Convergence, however, is relatively slow, as is shown by the numerical results of Table 3.17.

The key commands of the routine `Example3_59.m` are as follows:

```
ab=r_laguerre(n,m+1); ab(1,2)=ab(1,2)/prod(1:m);
xw=gauss(n,ab);
ta(1:n,1)=xw(:,1); ta(1:n,2)=xw(:,2)./(xw(:,1).^(m+1));
x=linspace(0,ta(n,1));
errmax=max(abs(splinefunc(n,m,x,ta)-exp(-x)));
```

The routine `splinefunc.m` evaluates $s_{n,m}(x)$ for any vector-valued x and for knots t_ν and coefficients a_ν input through the $n \times 2$ array `ta`.

Example 3.60 The Maxwell distribution, revisited.

For $f(t) = \mathrm{e}^{-t^2}$, the measure (3.3.14) becomes

$$\mathrm{d}\lambda^{[m]}(t) = \frac{1}{m!}\, t^{m+1} H_{m+1}(t)\mathrm{e}^{-t^2}\,\mathrm{d}t \quad \text{on } \mathbb{R}_+,$$

where H_{m+1} is the Hermite polynomial of degree $m + 1$ (cf. Commentaries to Table 1.1). If, as we assume, $m > 0$, then H_{m+1} changes sign at least once on $\mathbb{R}_+$, so that $\mathrm{d}\lambda^{[m]}$ is no longer a positive measure. The existence of a Gauss quadrature formula (3.3.15) with distinct positive nodes is, therefore, in doubt, and thus also the existence of the respective spline approximant (3.3.12).

In order to explore these issues, we attempt to generate the three-term recurrence relation for the monic orthogonal polynomials $\pi_k(\,\cdot\,) = \pi_k(\,\cdot\,;\mathrm{d}\lambda^{[m]})$,

$$\pi_{k+1}(t) = (t - \alpha_k(\mathrm{d}\lambda^{[m]}))\pi_k(t) - \beta_k(\mathrm{d}\lambda^{[m]})\pi_{k-1}(t). \tag{3.3.25}$$

They exist uniquely as long as the β-coefficients do not vanish. (We can no longer expect them to be positive, however.) Since the inner product is

$$(u, v)_{\mathrm{d}\lambda^{[m]}} = \frac{1}{m!} \int_{\mathbb{R}_+} u(t)v(t)t^{m+1}H_{m+1}(t)\mathrm{e}^{-t^2}\,\mathrm{d}t,$$

that is, up to a polynomial factor of degree $2m + 2$, the one for the half-range Hermite measure, it is relatively straightforward to implement the discretization

method of §2.2.4, using Gauss quadrature formulae for the half-range Hermite measure to do the discretizations. The procedure furnishes exact answers if we use an $(n+m+1)$-point quadrature rule, assuming we want the first n recurrence coefficients. The quadrature rule in question, on the other hand, can be generated in the usual way (cf. §3.1.1.1) from the first $n+m+1$ half-range Hermite recurrence coefficients, which, in turn, are computable as described in Example 2.41. (The first 100 of them are available to 25 decimal places in the `OPQ` file `abhrhermite`.)

If $\beta_k = \beta_k(\mathrm{d}\lambda^{[m]}) \neq 0$ for $k = 0, 1, \ldots, n$, the desired Gauss nodes τ_ν^G are the eigenvalues of the (nonsymmetric) Jacobi matrix

$$\tilde{\boldsymbol{J}}_n(\mathrm{d}\lambda^{[m]}) = \begin{bmatrix} \alpha_0 & 1 & & & \mathbf{0} \\ \beta_1 & \alpha_1 & 1 & & \\ & \beta_2 & \alpha_2 & \ddots & \\ & & \ddots & \ddots & 1 \\ \mathbf{0} & & & \beta_{n-1} & \alpha_{n-1} \end{bmatrix}. \tag{3.3.26}$$

Since some of the βs may well be negative, we are not attempting to symmetrize the matrix as is customarily done for positive measures. It is still true, however, that our spline approximation problem has a unique solution if and only if all eigenvalues of (3.3.26) are simple and positive. In that case, we can proceed to compute the required Gauss weights λ_ν^G. By putting $g(t) = \pi_{\mu-1}(t; \mathrm{d}\lambda^{[m]})$, $\mu = 1, 2, \ldots, n$, in (3.3.15), it is easily seen that the vector $\boldsymbol{\lambda}^G = [\lambda_1^G, \lambda_2^G, \ldots, \lambda_n^G]^{\mathrm{T}}$ is the solution of the linear system

$$\boldsymbol{P}_n(\mathrm{d}\lambda^{[m]})\boldsymbol{\lambda}^G = \beta_0 \boldsymbol{e}_1, \quad \boldsymbol{e}_1^{\mathrm{T}} = [1, 0, \ldots, 0], \tag{3.3.27}$$

where $\boldsymbol{P}_n$ is the matrix whose element in position (μ, ν) is $\pi_{\mu-1}(\tau_\nu^G)$, $\mu, \nu = 1, 2, \ldots, n$.

The computations were carried out for $n = 1:20$ and $m = 1:3$ (see the `OPQ` routine `Example3_60.m`). All coefficients β_k were found to be different from zero, but quite a few of them negative; see Table 3.18. Interestingly, the negative βs seem to occur in pairs of two.

Table 3.18 *The signs of the coefficients β_k in (3.3.25).*

m	$\beta_k < 0$ for $k =$
1	2–3, 6–7, 10–11, 15–16
2	1–2, 4–5, 7–8, 11–12, 14–15, 18–19
3	1–2, 4–5, 9–10, 16–17

In case all eigenvalues of the Jacobi matrix (3.3.26) are positive, we can take them as the nodes t_ν of the spline (3.3.12) and obtain the coefficients a_ν by means of (3.3.16) in terms of the solution $\boldsymbol{\lambda}^G$ of (3.3.27). A summary of the results is

Table 3.19 *Existence and accuracy of the spline approximations of Example 3.60.*

n	$m=1$	$m=2$	$m=3$	n	$m=1$	$m=2$	$m=3$
1	6.9(–2)	1.8(–1)	2.6(–1)	11	—	1.1(–3)	1.1(–4)
2	8.2(–2)	—	2.3(–1)	12	—	—	*
3	—	1.1(–2)	2.5(–3)	13	7.8(–3)	6.7(–4)	*
4	3.5(–2)	6.7(–3)	2.2(–3)	14	8.3(–3)	5.6(–4)	8.1(–5)
5	2.6(–2)	—	1.6(–3)	15	7.7(–3)	—	7.1(–5)
6	2.2(–2)	3.1(–3)	*	16	—	4.9(–4)	7.8(–5)
7	—	2.4(–3)	*	17	—	3.8(–4)	3.8(–5)
8	1.4(–2)	—	3.4(–4)	18	5.5(–3)	3.8(–4)	*
9	1.1(–2)	1.7(–3)	2.5(–4)	19	5.3(–3)	—	*
10	9.0(–3)	1.1(–3)	—	20	5.4(–3)	3.1(–4)	*

presented in Table 3.19. A dash indicates the presence of a negative eigenvalue and an asterisk the presence of a pair of conjugate complex eigenvalues. In all cases computed, there were never more than one negative eigenvalue, or more than one pair of complex eigenvalues. The numbers shown in Table 3.19 represent $\|s_{n,m} - f\|_\infty$ computed as in Example 3.59. In the case $n = 16$, $m = 3$, the matrix $\boldsymbol{P}_n$ is close to singular and, therefore, the corresponding entry in Table 3.19 possibly inaccurate.

3.3.2 *Approximation on a compact interval*

We consider now moment-preserving spline approximation on a finite interval, which, without loss of generality, may be assumed to be the interval $[0, 1]$. The spline function $s_{n,m}$ then has an additional polynomial component, so that

$$s_{n,m}(t) = p(t) + \sum_{\nu=1}^{n} a_\nu (t_\nu - t)_+^m, \quad p \in \mathbb{P}_m, \quad 0 \le t \le 1, \tag{3.3.28}$$

and we assume that all knots t_ν are strictly inside the interval $[0, 1]$,

$$0 < t_1 < t_2 < \cdots < t_n < 1. \tag{3.3.29}$$

There are two approximation problems that seem worth considering.

Problem I. Find $s_{n,m}$ in (3.3.28) such that

$$\int_0^1 s_{n,m}(t) t^j \, \mathrm{d}t = \mu_j, \quad j = 0, 1, \ldots, 2n + m. \tag{3.3.30}$$

Compared to (3.3.13), we can match $m + 1$ additional moments, since we have that many more parameters (the coefficients of p) at our disposal.

Problem II. Find $s_{n,m}$ in (3.3.28) such that

$$\int_0^1 s_{n,m}(t) t^j \, \mathrm{d}t = \mu_j, \quad j = 0, 1, \ldots, 2n - 1, \tag{3.3.31}$$

and

$$s_{n,m}^{(\mu)}(1) = f^{(\mu)}(1), \quad \mu = 0, 1, \ldots, m. \tag{3.3.32}$$

Here, we must assume that the first m derivatives of f at the end point $t = 1$ exist and are known. These immediately determine p, since $s_{n,m}^{(\mu)}(1) = p^{(\mu)}(1)$.

If f is a polynomial of degree m, then $s_{n,m} = f$ is a trivial solution of either problem. We will, therefore, assume that $f \notin \mathbb{P}_m$.

Theorem 3.61 *Assume that $f \in C^{m+1}[0,1]$ and $f \notin \mathbb{P}_m$. Then, Problem I has a unique solution if and only if the measure*

$$\mathrm{d}\lambda^{[m]}(t) = \frac{(-1)^{m+1}}{m!} f^{(m+1)}(t)\,\mathrm{d}t \quad \textit{on } [0,1] \tag{3.3.33}$$

admits a generalized Gauss–Lobatto quadrature formula (cf. §3.1.1.4)

$$\begin{aligned}\int_0^1 g(t)\,\mathrm{d}\lambda^{[m]}(t) = &\sum_{\mu=0}^{m}[\lambda_0^{(\mu)} g^{(\mu)}(0) + (-1)^{\mu}\lambda_{n+1}^{(\mu)} g^{(\mu)}(1)] \\ &+ \sum_{\nu=1}^{n} \lambda_\nu^L g(\tau_\nu^L) \quad \textit{for all } g \in \mathbb{P}_{2n+2m+1},\end{aligned} \tag{3.3.34}$$

satisfying $0 < \tau_1^L < \tau_2^L < \cdots < \tau_n^L < 1$. If that is the case, the knots t_ν and coefficients a_ν in (3.3.28) are given by

$$t_\nu = \tau_\nu^L, \quad a_\nu = \lambda_\nu^L, \quad \nu = 1, 2, \ldots, n, \tag{3.3.35}$$

and the polynomial p in (3.3.28) is uniquely determined by its derivative values at $t = 1$ given by

$$p^{(\mu)}(1) = f^{(\mu)}(1) + (-1)^m m!\lambda_{n+1}^{(m-\mu)}, \quad \mu = 0, 1, \ldots, m. \tag{3.3.36}$$

Proof See Frontini, Gautschi, and Milovanović (1987, §2.2, Corollary 1 to Theorem 2.3). □

Note that complete monotonicity of f (cf. the paragraph preceding Theorem 3.58) again implies positivity of $\mathrm{d}\lambda^{[m]}$, hence the unique existence of $s_{n,m}$ for any $n \geq 1$ and $m \geq 0$. In turn, by Theorem 3.12 this implies $a_\nu > 0$ in (3.3.28), but complete monotonicity of $s_{n,m}$ (in the weak sense) only if $(-1)^k p^{(k)}(t) \geq 0$ for all k. Since by Taylor's theorem

$$(-1)^k p^{(k)}(t) = (-1)^k \left(\sum_{\mu=0}^{m} (-1)^{\mu} \frac{p^{(\mu)}(1)}{\mu!} (1-t)^{\mu} \right)^{(k)},$$

the latter is true if $(-1)^{\mu} p^{(\mu)}(1) \geq 0$ for $\mu = 0, 1, \ldots, m$, or, by (3.3.36), if

$$(-1)^{\mu} f^{(\mu)}(1) + m!(-1)^{m-\mu}\lambda_{n+1}^{(m-\mu)} \geq 0, \quad \mu = 0, 1, \ldots, m.$$

Since the first term is positive by assumption, these inequalities restrict only those weights in (3.3.34) for which $(-1)^{\rho}\lambda_{n+1}^{(\rho)} < 0$.

Theorem 3.62 *Assume that $f \in C^{m+1}[0,1]$ and $f \notin \mathbb{P}_m$. Then, Problem II has a unique solution if and only if the measure $\mathrm{d}\lambda^{[m]}$ in (3.3.33) admits a generalized Gauss–Radau quadrature formula* (cf. §3.1.1.4)

$$\int_0^1 g(t)\,\mathrm{d}\lambda^{[m]}(t) = \sum_{\mu=0}^{m} \lambda_0^{(\mu)} g^{(\mu)}(0) + \sum_{\nu=1}^{n} \lambda_\nu^R g(\tau_\nu^R) \quad \textit{for all } g \in \mathbb{P}_{2n+m}, \tag{3.3.37}$$

satisfying $0 < \tau_1^R < \tau_2^R < \cdots < \tau_n^R < 1$. If that is the case, the knots t_ν and coefficients a_ν in (3.3.28) are given by

$$t_\nu = \tau_\nu^R, \quad a_\nu = \lambda_\nu^R, \quad \nu = 1, 2, \ldots, n, \tag{3.3.38}$$

and (trivially)

$$p(t) = \sum_{\mu=0}^{m} \frac{f^{(\mu)}(1)}{\mu!}\,(t-1)^\mu. \tag{3.3.39}$$

Proof See Frontini, Gautschi, and Milovanović (1987, §2.2, Corollary 1 to Theorem 2.4). □

Complete monotonicity of f, as before, implies the unique existence of $s_{n,m}$ for all n and m, but now also complete monotonicity (in the weak sense) of each $s_{n,m}$.

There are error estimates in terms of the remainder terms of the generalized Gauss–Lobatto and Gauss–Radau quadrature rules that are entirely analogous to the one in Theorem 3.58. For this, as well as for convergence results as $n \to \infty$ and numerical examples, we refer to Frontini, Gautschi, and Milovanović (1987, §3 and 4).

3.4 Slowly convergent series

There are many ways slowly convergent series can be evaluated. A large class of methods is based on linear or nonlinear sequence transformations, that is, the sequence of partial sums of the series is transformed into another sequence that converges faster to the same limit. For texts along these lines, see, for example, Wimp (1981), Delahaye (1988), and Brezinski and Redivo Zaglia (1991). An alternative approach, more in the spirit of this book, consists in first representing the series as a definite integral involving a positive measure, and then applying Gaussian quadrature to the integral. This also produces a new sequence—the sequence of Gauss quadrature approximations—but it originates from the integral representation of the series and not from its partial sums. In the following, we consider simple examples of this idea, involving series

$$S = \sum_{k=1}^{\infty} a_k \tag{3.4.1}$$

whose general term is expressible in terms of the Laplace transform, or its derivative, of a known function.

3.4.1 *Series generated by a Laplace transform*

We assume that the term a_k in the series (3.4.1) is the Laplace transform

$$(\mathcal{L}f)(s) = \int_0^\infty \mathrm{e}^{-st} f(t)\,\mathrm{d}t \tag{3.4.2}$$

evaluated at $s = k$ of some known function f,

$$a_k = (\mathcal{L}f)(k), \quad k = 1, 2, 3, \dots\ . \tag{3.4.3}$$

Such series typically converge slowly. For example, if $f \sim t^\sigma$, $\sigma > 0$, as $t \to 0$, and f grows at most exponentially at infinity, one has by Watson's Lemma (see, e.g. Wong (1989, p. 20)) that $a_k \sim k^{-\sigma-1}$ as $k \to \infty$, showing slow convergence of (3.4.1) unless σ is large. We can write, however,

$$S = \sum_{k=1}^\infty (\mathcal{L}f)(k) = \sum_{k=1}^\infty \int_0^\infty \mathrm{e}^{-kt} f(t)\,\mathrm{d}t,$$

and, upon interchanging summation with integration and some minor regrouping,

$$S = \int_0^\infty \sum_{k=1}^\infty \mathrm{e}^{-(k-1)t} \cdot \mathrm{e}^{-t} f(t)\,\mathrm{d}t = \int_0^\infty \frac{1}{1-\mathrm{e}^{-t}}\,\mathrm{e}^{-t} f(t)\,\mathrm{d}t,$$

that is,

$$S = \int_0^\infty \frac{t}{1-\mathrm{e}^{-t}}\,\frac{f(t)}{t}\,\mathrm{e}^{-t}\,\mathrm{d}t. \tag{3.4.4}$$

This is the desired integral representation of the series. If the series converges at least as fast as $\sum k^{-\nu-1}$, $\nu > 0$, then $f(t)/t$ in (3.4.4) is integrable at $t = 0$.

The task is now shifted from one of summation to one of integration. There are, in fact, several ways we can proceed. One that comes to mind immediately is Gauss–Laguerre quadrature of

$$\frac{t}{1-\mathrm{e}^{-t}}\,\frac{f(t)}{t}$$

in (3.4.4) or, possibly, generalized Gauss–Laguerre quadrature if $f(t)/t$ is not regular at $t = 0$. On the surface, this seems like a natural approach, but it ignores the presence of poles (located at the integer multiples of $2\pi\mathrm{i}$) in the first factor of the integrand. These poles have the effect of slowing down convergence of Gauss–Laguerre quadrature. A better way is to incorporate these poles (or at least some of them) into a rational Gauss–Laguerre formula of the kind discussed in §3.1.4.1, Example 3.27, where $\xi_\nu = 0$ and $\eta_\nu = 1/(2\nu\pi)$. (Experience gained in §3.1.4.3 suggests incorporating the first $m = 2\lfloor (n+1)/2 \rfloor$ poles in the n-point

quadrature rule.) Alternatively, they can be integrated, as in Example 2.42, into an Einstein weight function by writing

$$S = \int_0^\infty \frac{f(t)}{t}\,\mathrm{d}\lambda(t), \quad \mathrm{d}\lambda(t) = \frac{t}{\mathrm{e}^t - 1}\,\mathrm{d}t. \tag{3.4.5}$$

Then, if $f(t)/t$ is a smooth function, the correponding Gauss–Einstein quadrature rule converges rapidly. If $f(t)/t \sim t^{\nu-1}$, $\nu > 0$, as $t \to 0$, then modified Gauss–Einstein quadrature (cf. Example 2.43) is called for.

Example 3.63 The *Theodorus constant*

$$T = \sum_{k=1}^{\infty} \frac{1}{k^{3/2} + k^{1/2}} = 1.860025079221190307\ldots\ .$$

So called by Davis (1993) because of its relation to a spiral attributed to the ancient Greek mathematician Theodorus of Cyrene, it is an example of (3.4.3). Indeed,

$$\frac{1}{s^{3/2} + s^{1/2}} = s^{-1/2}\frac{1}{s+1}\,,$$

so that the Convolution Theorem for Laplace transforms can be applied if one notes that $s^{-1/2} = (\mathcal{L}1/\sqrt{\pi t})(s)$ and $(s+1)^{-1} = (\mathcal{L}\mathrm{e}^{-t})(s)$,

$$s^{-1/2}(s+1)^{-1} = \left(\mathcal{L}\frac{1}{\sqrt{\pi t}} * \mathrm{e}^{-t}\right)(s).$$

Here, the star indicates convolution,

$$\frac{1}{\sqrt{\pi t}} * \mathrm{e}^{-t} = \int_0^t \frac{1}{\sqrt{\pi\tau}}\,\mathrm{e}^{-(t-\tau)}\,\mathrm{d}t = \frac{\mathrm{e}^{-t}}{\sqrt{\pi}}\int_0^t \frac{\mathrm{e}^{\tau}}{\sqrt{\tau}}\,\mathrm{d}\tau.$$

Substituting $\tau = u^2$, one gets

$$\frac{1}{\sqrt{\pi t}} * \mathrm{e}^{-t} = \frac{2}{\sqrt{\pi}}\,\mathrm{e}^{-t}\int_0^{\sqrt{t}} \mathrm{e}^{u^2}\,\mathrm{d}u$$

and, therefore,

$$f(t) = \frac{2}{\sqrt{\pi}}\,F(\sqrt{t}),$$

where

$$F(x) = \mathrm{e}^{-x^2}\int_0^x \mathrm{e}^{t^2}\,\mathrm{d}t$$

is Dawson's integral (cf. Abramowitz and Stegun (1992, Chapter 7)).

The integral representation for T can now be written in the form

$$T = \frac{2}{\sqrt{\pi}} \int_0^\infty \frac{t}{1 - \mathrm{e}^{-t}} \frac{F(\sqrt{t})}{\sqrt{t}}\, t^{-1/2} \mathrm{e}^{-t}\, \mathrm{d}t \tag{3.4.6}$$

or, alternatively, as

$$T = \frac{2}{\sqrt{\pi}} \int_0^\infty \frac{F(\sqrt{t})}{\sqrt{t}}\, t^{-1/2}\, \mathrm{d}\lambda(t), \quad \mathrm{d}\lambda(t) = \frac{t}{\mathrm{e}^t - 1}\, \mathrm{d}t. \tag{3.4.7}$$

The three quadrature schemes mentioned above—generalized Gauss–Laguerre and rational Gauss–Laguerre quadrature of (3.4.6), and modified (by $t^{-1/2}$) Gauss–Einstein quadrature of (3.4.7)—are compared with respect to relative errors in Table 3.20; see the `OPQ` routine `Example3_63.m`.

Table 3.20 *Relative errors of three quadrature schemes to evaluate the Theodorus constant.*

n	Gauss–Laguerre	Rational Gauss–Laguerre	Gauss–Einstein
1	9.6799(–03)	1.5635(–02)	1.3610(–01)
4	5.5952(–06)	1.1893(–08)	2.1735(–04)
7	4.0004(–08)	5.9689(–16)	3.3459(–07)
10	5.9256(–10)		5.0254(–10)
15	8.2683(–12)		9.4308(–15)
20	8.9175(–14)		4.7751(–16)
	Timing: 10.8	Timing: 8.78	Timing: 10.4

It is seen that rational Gauss–Laguerre quadrature is the clear winner, followed, at a distance, by Gauss–Einstein and ordinary Gauss–Laguerre quadratures. This is true not only in terms of accuracy, but also in terms of machine time, the timing for rational Gauss–Laguerre being, as shown, about 80% of the one for the other quadrature schemes.

Example 3.64 The *Hardy–Littlewood function*

$$H(x) = \sum_{k=1}^{\infty} \frac{1}{k} \sin \frac{x}{k}, \quad x > 0.$$

This function has an interesting history. It was introduced by Hardy and Littlewood (1936) in connection with a summation procedure of Lambert. Hardy and Littlewood showed that there are infinitely many (though rare) values of x with $x \to \infty$ such that $H(x) > C(\log\log x)^{1/2}$. The function, therefore, is unbounded from above. Recently, Clark and Ismail (2003) studied the complete monotonicity on $[0, \infty]$ of the function $-(x^m \psi^{(m)}(x))^{(m)}$, where ψ is the logarithmic derivative of the gamma function. They proved complete monotonicity for $m = 1, 2, \ldots, 16$ and conjectured it to hold for all m. The conjecture was

shown by Alzer, Berg, and Koumandos (2004) to be equivalent to $H(x) > -\pi/2$ on $[0, \infty]$, and eventually disproved by showing that $H(x) < -C(\log\log x)^{1/2}$ for infinitely many (but rare) values of x going to infinity.

To express the general term of the series as a Laplace transform, we recall (Abramowitz and Stegun, 1992, eqn 29.3.81) that

$$\frac{1}{s}\,\mathrm{e}^{x/s} = \left(\mathcal{L}_{(t)} I_0(2\sqrt{xt})\right)(s), \tag{3.4.8}$$

where I_0 is the modified Bessel function of order zero. Therefore, by Euler's formula,

$$\frac{1}{s}\,\sin(x/s) = \frac{1}{s}\,\frac{1}{2\mathrm{i}}\,(\mathrm{e}^{\mathrm{i}x/s} - \mathrm{e}^{-\mathrm{i}x/s}) = \frac{1}{2\mathrm{i}}\,\left(\mathcal{L}_{(t)}[I_0(2\sqrt{\mathrm{i}xt}) - I_0(2\sqrt{-\mathrm{i}xt})](s)\right),$$

so that

$$f(t) = f(t;x) = \frac{1}{2\mathrm{i}}\,[I_0(2\sqrt{\mathrm{i}xt}) - I_0(2\sqrt{-\mathrm{i}xt})]. \tag{3.4.9}$$

This is an entire function of $u = xt$, and it is readily seen from its power series expansion that $\lim_{t\to 0} f(t;x)/t = x$. For purposes of calculation, however, the power series is of limited use, since it suffers from severe cancellation of terms when $u = xt$ is large.

A more suitable expression for f can be obtained from the integral representation (cf. Abramowitz and Stegun (1992, eqn 9.6.16))

$$I_0(z) = \frac{1}{\pi}\,\int_0^\pi \mathrm{e}^{z\cos\theta}\,\mathrm{d}\theta,$$

which, substituted in (3.4.9), yields

$$f(t;x) = \frac{1}{\pi}\,\int_0^\pi \mathrm{e}^{\sqrt{2u}\cos\theta}\,\sin(\sqrt{2u}\cos\theta)\,\mathrm{d}\theta, \quad u = xt. \tag{3.4.10}$$

Since the integrand is a 2π-periodic, even, and entire function of θ, integration in (3.4.10) is in effect over the full period, and the composite trapezoidal rule the method of choice for evaluating the integral. See the `OPQ` routine `fHL.m`.

In analogy to (3.4.4) and (3.4.5), we now have

$$H(x) = \int_0^\infty \frac{t}{1-\mathrm{e}^{-t}}\,\frac{f(t;x)}{t}\,\mathrm{e}^{-t}\,\mathrm{d}t$$

or

$$H(x) = \int_0^\infty \frac{f(t;x)}{t}\,\mathrm{d}\lambda(t), \quad \mathrm{d}\lambda(t) = \frac{t}{\mathrm{e}^t - 1}\,\mathrm{d}t,$$

and the same three methods as in Example 3.63 can be used to evaluate these integrals. The third one—Gauss–Einstein quadrature—is now performing best, both with regard to speed of convergence and machine time, but shares with the

other two methods their propensity of losing accuracy owing to cancellation of terms in the quadrature sum. A measure of cancellation is the absolutely largest term of the quadrature rule divided by the absolute value of the quadrature sum. This measure is shown in the column of Table 3.21 headed by "can." The smallest integer n for which two consecutive quadrature approximations (with n resp.

Table 3.21 *Performance of three quadrature schemes to evaluate the Hardy–Littlewood function.*

x	n	$H(x)$	can	Nf
		Gauss–Laguerre		
1	10	1.472828	3.780(–01)	30
5	13	0.944182	2.956(+00)	40
10	20	0.759295	2.377(+01)	50
20	28	2.197003	1.299(+03)	60
40	45	2.970698	1.893(+07)	70
Timing: 24.7				
		Rational Gauss–Laguerre		
1	7	1.472828	4.080(–01)	30
5	12	0.944182	2.507(+00)	40
10	16	0.759295	2.415(+01)	40
20	25	2.197003	1.279(+03)	50
40	49	2.970699	1.579(+07)	80
Timing: 487.3				
		Gauss–Einstein		
1	5	1.472828	5.017(–01)	30
5	9	0.944182	3.596(+00)	40
10	13	0.759295	3.569(+01)	40
20	21	2.197003	1.359(+03)	60
40	39	2.970699	1.689(+07)	70
Timing: 16.0				

$n+1$ terms) differ in absolute value by less than $\varepsilon_0 = 10^9 \times \texttt{eps} = 2.22 \times 10^{-7}$ are shown in the column headed by "n." The last column shows how many terms (in steps of 10) are needed in the composite trapezoidal rule to obtain the function f in (3.4.10) within an error of $\varepsilon_1 = 10^3 \times \texttt{eps} = 2.22 \times 10^{-13}$. The rational Gauss–Laguerre method, when $x = 40$, experiences overflow problems in the routine `stieltjes.m` used in `mcdis.m` for generating the rational quadrature rule. To eliminate them, we used the routine `lanczos.m` in place of `stieltjes.m`, paying the heavy price associated with this choice already noted in Examples 2.39 and 2.40. The results in Table 3.21, showing the superiority of Gauss–Einstein quadrature, are produced by the routine `Example3_64.m`. For a graph of $H(x)$ for $0 \le x \le 100$, see Figure 3.6.

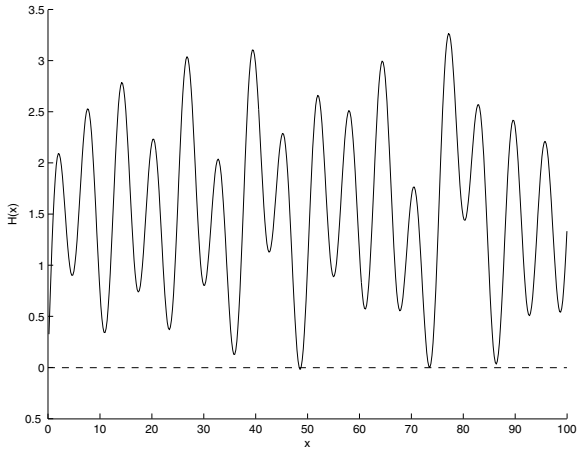

FIG. 3.6. The Hardy–Littlewood function on $[0, 100]$.

3.4.2 *"Alternating" series generated by a Laplace transform*

These are series (3.4.1) in which

$$a_k = (-1)^{k-1}(\mathcal{L}f)(k), \quad k = 1, 2, 3, \ldots, \tag{3.4.11}$$

that is, the signs of the Laplace transforms, not necessarily those of a_k, alternate. Here, in place of (3.4.4), one finds

$$S = \int_0^\infty \frac{1}{1 + \mathrm{e}^{-t}} f(t)\mathrm{e}^{-t}\,\mathrm{d}t. \tag{3.4.12}$$

We have the same three options as in §3.4.1 of evaluating this integral, the third one being based on

$$S = \int_0^\infty f(t)\,\mathrm{d}\lambda(t), \quad \mathrm{d}\lambda(t) = \frac{1}{\mathrm{e}^t + 1}\,\mathrm{d}t,$$

that is, on Gauss quadrature relative to a Fermi distribution (cf. §3.1.4.3).

Example 3.65 A logarithmic series $\sum_{k=1}^\infty (-1)^{k-1}(k+1)^{-1} = 1 - \ln 2$.

Since $(s+1)^{-1} = (\mathcal{L}\mathrm{e}^{-t})(s)$, we have $f(t) = \mathrm{e}^{-t}$ and $S = \int_0^\infty \mathrm{e}^{-t}\,\mathrm{d}t/(\mathrm{e}^t + 1)$. The `OPQ` routine `Example3_65.m` implements the three quadrature methods. The results are summarized in Table 3.22, showing relative errors and timings.

It is seen that ordinary Gauss–Laguerre quadrature is rather slow in converging, more so than in the preceding examples because of the poles of the integrand being at integer multiples of $\pi\mathrm{i}$ rather than $2\pi\mathrm{i}$ as before. In contrast, rational Gauss–Laguerre converges quite fast, but is more costly. Gauss–Fermi quadrature, converging reasonably fast and being also exceptionally fast in terms of machine time, appears to be a good compromise.

Table 3.22 *Relative errors of three quadrature schemes to evaluate the logarithmic series of Example 3.65.*

n	Gauss–Laguerre	Rational Gauss–Laguerre	Gauss–Fermi
1	1.2355(–01)	6.1564(–02)	3.1044(–01)
4	7.6210(–05)	1.2730(–06)	9.2350(–04)
7	9.8184(–06)	1.9494(–11)	1.7364(–06)
10	3.2281(–06)	9.0452(–16)	2.9055(–09)
15	6.4151(–08)		6.1689(–14)
20	4.3124(–09)		1.9090(–16)
35	6.1327(–13)		
50	4.5226(–15)		
	Timing: 6.95	Timing: 19.3	Timing: 1.59

Example 3.66 The series $\sum_{k=1}^{\infty}(-1)^{k-1}k^{-1}\mathrm{e}^{-1/k} = 0.19710793639795065\ldots$.

From (3.4.8) one obtains $s^{-1}\mathrm{e}^{-1/s} = (\mathcal{L}J_0(2\sqrt{t}))(s)$, so that $f(t) = J_0(2\sqrt{t})$, and, therefore,

$$S = \int_0^{\infty} \frac{1}{1+\mathrm{e}^{-t}}\, J_0(2\sqrt{t})\mathrm{e}^{-t}\,\mathrm{d}t,$$

or

$$S = \int_0^{\infty} J_0(2\sqrt{t})\,\mathrm{d}\lambda(t), \quad \mathrm{d}\lambda(t) = \frac{1}{\mathrm{e}^t+1}\,\mathrm{d}t.$$

The `OPQ` routine `Example3_66.m`, a slight variation of `Example3_65.m`, produces results as shown in Table 3.23. They are similar to those in Table 3.22 except for Gauss–Fermi quadrature, which is now the most efficient in all respects.

Table 3.23 *Relative errors of three quadrature schemes to evaluate the series of Example 3.66.*

n	Gauss–Laguerre	Rational Gauss–Laguerre	Gauss–Fermi
1	1.6961(–01)	1.0310(–01)	5.6994(–01)
4	4.4754(–03)	4.6605(–05)	9.6454(–07)
7	1.7468(–04)	1.8274(–09)	9.1529(–15)
10	3.7891(–06)	1.5729(–13)	2.8163(–16)
15	2.6569(–07)	1.5490(–15)	
20	8.6155(–09)		
40	1.8066(–13)		
	Timing: 12.7	Timing: 19.5	Timing: 4.95

3.4.3 *Series generated by the derivative of a Laplace transform*

We now consider the case where

$$a_k = -\left.\frac{\mathrm{d}}{\mathrm{d}s}\,(\mathcal{L}f)(s)\right|_{s=k}, \quad k = 1, 2, 3, \ldots\ . \tag{3.4.13}$$

A short calculation similar to the one leading to (3.4.4) will show in this case that

$$S = \int_0^\infty \frac{t}{1-\mathrm{e}^{-t}}\, f(t)\mathrm{e}^{-t}\,\mathrm{d}t, \tag{3.4.14}$$

or, alternatively,

$$S = \int_0^\infty f(t)\,\mathrm{d}\lambda(t), \quad \mathrm{d}\lambda(t) = \frac{t}{\mathrm{e}^t-1}\,\mathrm{d}t, \tag{3.4.15}$$

that is, integration relative to the Einstein measure. The three quadature methods used previously continue to be applicable.

Example 3.67 The series $\sum_{k=1}^\infty (k-1)k^{-3}\mathrm{e}^{-1/k} = 0.34291894384460978\ldots$.

The general term in this series is the negative derivative of the Laplace transform used in Example 3.66, so that again $f(t) = J_0(2\sqrt{t})$ and

$$S = \int_0^\infty \frac{t}{1-\mathrm{e}^{-t}}\, J_0(2\sqrt{t})\mathrm{e}^{-t}\,\mathrm{d}t$$

or

$$S = \int_0^\infty J_0(2\sqrt{t})\,\mathrm{d}\lambda(t), \quad \mathrm{d}\lambda(t) = \frac{t}{\mathrm{e}^t-1}\,\mathrm{d}t.$$

The performance of the three quadrature methods, not surprisingly, is similar to the one shown in Table 3.23; see the `OPQ` routine `Example3_67.m` for details.

Example 3.68 The series $\sum_{k=1}^\infty (\frac{3}{2}k+1)k^{-2}(k+1)^{-3/2} = 1.2859748161552402\ldots$.

It is known (Abramowitz and Stegun, 1992, eqn 29.3.44) that

$$(\mathcal{L}\,\mathrm{erf}\sqrt{t})(s) = \frac{1}{s}\,\frac{1}{\sqrt{s+1}}\,,$$

the negative derivative of which, for $s = k$, yields the general term of the series. Thus, $f(t) = \mathrm{erf}\sqrt{t}$, and

$$S = \int_0^\infty \frac{t}{1-\mathrm{e}^{-t}}\,\mathrm{erf}\sqrt{t}\,\mathrm{e}^{-t}\,\mathrm{d}t.$$

To remove the square-root singularity at $t = 0$, we write this as

$$S = \int_0^\infty \frac{t}{1-\mathrm{e}^{-t}}\,\frac{\mathrm{erf}\sqrt{t}}{\sqrt{t}}\,t^{1/2}\mathrm{e}^{-t}\,\mathrm{d}t,$$

or else as

$$S = \int_0^\infty \frac{\mathrm{erf}\sqrt{t}}{\sqrt{t}}\,t^{1/2}\,\mathrm{d}\lambda(t), \quad \mathrm{d}\lambda(t) = \frac{t}{\mathrm{e}^t-1}\,\mathrm{d}t.$$

To evaluate this effectively requires the generalized Laguerre measure (with parameter $\alpha = \frac{1}{2}$) in the former, and the modified (by $t^{1/2}$) Einstein measure in the latter integral. Modified in this manner, the three quadrature methods used in the previous examples perform as expected. See Table 3.24 for numerical results, and the `OPQ` routine `Example3_68.m` for implementational details.

Table 3.24 *Relative errors of three quadrature schemes to evaluate the series of Example 3.68.*

n	Gauss–Laguerre	Rational Gauss–Laguerre	Gauss–Einstein
1	4.0125(–03)	5.1071(–02)	8.1715(–02)
4	1.5108(–05)	4.5309(–08)	1.6872(–04)
7	4.6576(–08)	1.3226(–13)	3.1571(–07)
10	3.0433(–09)	1.2087(–15)	5.4661(–10)
15	4.3126(–11)		1.2605(–14)
20	7.6664(–14)		
30	3.4533(–16)		
	Timing: 6.50	Timing: 10.8	Timing: 1.58

3.4.4 *"Alternating" series generated by the derivative of a Laplace transform*

This is the case of

$$a_k = -(-1)^{k-1}\frac{\mathrm{d}}{\mathrm{d}s}\,(\mathcal{L}f)(s)\bigg|_{s=k}, \quad k = 1, 2, 3, \ldots, \tag{3.4.16}$$

which gives rise to

$$S = \int_0^\infty \frac{t}{1+\mathrm{e}^{-t}}\, f(t)\mathrm{e}^{-t}\,\mathrm{d}t \tag{3.4.17}$$

or

$$S = \int_0^\infty t f(t)\,\mathrm{d}\lambda(t), \quad \mathrm{d}\lambda(t) = \frac{1}{\mathrm{e}^t+1}\,\mathrm{d}t. \tag{3.4.18}$$

Example 3.69 The series

$$\sum_{k=1}^{\infty}(-1)^{k-1}(\tfrac{3}{2}+1)k^{-2}(k+1)^{-3/2} = 0.74288076461170605\ldots\ .$$

This is the alternating counterpart of the series in Example 3.68, hence again $f(t) = \operatorname{erf}\sqrt{t}$. With the same adjustments made as in Example 3.68 to take care of the square-root singularity, we need to evaluate

$$S = \int_0^\infty \frac{\sqrt{t}\operatorname{erf}\sqrt{t}}{1+\mathrm{e}^{-t}}\, t^{1/2}\mathrm{e}^{-t}\,\mathrm{d}t$$

and

$$S = \int_0^\infty \sqrt{t}\operatorname{erf}\sqrt{t}\cdot t^{1/2}\,\mathrm{d}\lambda(t), \quad \mathrm{d}\lambda(t) = \frac{1}{\mathrm{e}^t+1}\,\mathrm{d}t.$$

This is done as before, using, however, generalized ordinary and rational Gauss–Laguerre quadrature for the first of these integrals, and modified (by $t^{1/2}$) Gauss–Fermi quadrature for the second. Implemented in the `OPQ` routine `Example3_69.m`, the results are similar to those in Table 3.24, except that the first quadrature rule (generalized Gauss–Laguerre) requires $n = 50$ to reach an accuracy near the level of machine precision.

3.4.5 *Slowly convergent series occurring in plate contact problems*

The series to be considered here are series of the type

$$R_p(z) = \sum_{k=0}^{\infty} \frac{z^{2k+1}}{(2k+1)^p} \tag{3.4.19}$$

or the type

$$S_p(z) = \sum_{k=0}^{\infty} (-1)^k \frac{z^{2k+1}}{(2k+1)^p}\,, \tag{3.4.20}$$

where

$$z \in \mathbb{C}, \quad |z| \le 1, \quad p = 2 \text{ or } 3. \tag{3.4.21}$$

Of particular interest is the case where $|z|$ is close or equal to 1, in which case both series converge very slowly. It suffices to concentrate on the first of these series, R_p, since $S_p(z) = \mathrm{i}R_p(-\mathrm{i}z)$. Attention, moreover, can be restricted to the first quadrant in the complex plane, since $R_p(-z) = -R_p(z)$ and $R_p(\overline{z}) = \overline{R_p(z)}$.

Series of the type (3.4.19) with

$$z = x,\ 0 < x \le 1 \quad \text{or} \quad z = \mathrm{e}^{\mathrm{i}\alpha},\ \alpha \in \mathbb{R} \tag{3.4.22}$$

occur in the mathematical treatment of unilateral plate contact problems. When $z = e^{\mathrm{i}\alpha}$ is on the unit circle, some of these series can be summed explicitly as Fourier series. For example, see Hansen (1975, eqns (17.2.16) and (14.2.21)),

$$\sum_{k=0}^{\infty} \frac{\cos(2k+1)\alpha}{(2k+1)^2} = \frac{1}{8}\,\pi(\pi - 2|\alpha|), \quad -\pi \le \alpha \le \pi, \tag{3.4.23}$$

or

$$\sum_{k=0}^{\infty} \frac{\sin(2k+1)\alpha}{(2k+1)^3} = \frac{1}{8}\,\pi\alpha(\pi - |\alpha|), \quad -\pi \le \alpha \le \pi, \tag{3.4.24}$$

and there are analogous formulae for the alternating series. When $z = 1$, the sum of (3.4.19) is expressible in terms of the Riemann zeta function (Abramowitz and Stegun, 1992, eqn 23.2.20),

$$R_p(1) = (1 - 2^{-p})\zeta(p), \tag{3.4.25}$$

whereas $S_2(1)$ is known as Catalan's constant, and $S_3(1) = \pi^3/32$.

3.4.5.1 *The summation procedure* We follow the same idea as described in §3.4.1 except that only a part of the general term of the series (3.4.19)—namely

the coefficient—is expressed as a Laplace transform (cf. Abramowitz and Stegun (1992, eqn 29.3.11)),

$$\frac{1}{(k+\frac{1}{2})^p} = (\mathcal{L}f)(k), \quad f(t) = \frac{1}{(p-1)!}\, t^{p-1}\mathrm{e}^{-t/2}. \tag{3.4.26}$$

Then,

$$\begin{aligned} R_p(z) &= \frac{z}{2^p}\sum_{k=0}^{\infty}\frac{z^{2k}}{(k+\frac{1}{2})^p} = \frac{z}{2^p}\sum_{k=0}^{\infty} z^{2k}\int_0^{\infty}\mathrm{e}^{-kt}\cdot\frac{t^{p-1}\mathrm{e}^{-t/2}}{(p-1)!}\,\mathrm{d}t \\ &= \frac{z}{2^p(p-1)!}\int_0^{\infty}\sum_{k=0}^{\infty}(z^2\mathrm{e}^{-t})^k\cdot t^{p-1}\mathrm{e}^{-t/2}\,\mathrm{d}t \\ &= \frac{z}{2^p(p-1)!}\int_0^{\infty}\frac{1}{1-z^2\mathrm{e}^{-t}}\,t^{p-1}\mathrm{e}^{-t/2}\,\mathrm{d}t, \end{aligned}$$

that is,

$$R_p(z) = \frac{z}{2^p(p-1)!}\int_0^{\infty}\frac{t^{p-1}\mathrm{e}^{t/2}}{\mathrm{e}^t - z^2}\,\mathrm{d}t. \tag{3.4.27}$$

We distinguish two cases.

Case 1: $z = 1$. In this case, (3.4.27) can be given the forms

$$R_p(1) = \frac{1}{2^p(p-1)!}\int_0^{\infty}\frac{t^{p-1}\mathrm{e}^{t/2}}{1-\mathrm{e}^{-t}}\,\mathrm{e}^{-t}\,\mathrm{d}t \tag{3.4.28}$$

or

$$R_p(1) = \frac{1}{2^p(p-1)!}\int_0^{\infty} t^{p-2}e^{t/2}\,\mathrm{d}\lambda(t), \quad \mathrm{d}\lambda(t) = \frac{t}{\mathrm{e}^t-1}\,\mathrm{d}t, \tag{3.4.29}$$

and the three quadrature methods of §3.4.1 again become applicable. Alternatively, we may use the explicit formula (3.4.25) in conjunction with tabulated values of the Riemann zeta function (cf., e.g. McLellan IV (1968)). In particular, $R_2(1) = \pi^2/8$.

Case 2: $z \neq 1$. Here we could proceed similarly as in Case 1 and write, for example,

$$R_p(z) = \frac{z}{2^p(p-1)!}\int_0^{\infty}\frac{\mathrm{e}^t-1}{\mathrm{e}^t-z^2}\,t^{p-2}\mathrm{e}^{t/2}\,\mathrm{d}\lambda(t).$$

Unfortunately, the first factor in the integrand is rather ill-behaved when $|z|$ is close to 1, exhibiting a steep boundary layer near $t = 0$. Gaussian quadrature, therefore, will no longer be effective.

Instead, we make the change of variable $\mathrm{e}^{-t} = \tau$ in (3.4.27) (and then replace τ again by t) to obtain

$$R_p(z) = \frac{1}{2^p(p-1)!z}\int_0^1\frac{t^{-1/2}[\ln(1/t)]^{p-1}}{z^{-2}-t}\,\mathrm{d}t. \tag{3.4.30}$$

This expresses $R_p(z)$ as a Cauchy integral of the measure

$$\mathrm{d}\lambda^{[p]}(t) = t^{-1/2}[\ln(1/t)]^{p-1}\,\mathrm{d}t \tag{3.4.31}$$

(cf. (2.3.1) and (2.3.2)). Since under our assumptions z^{-2} lies outside of the interval $[0,1]$, the integral in (3.4.30) can be evaluated by the continued fraction algorithm of §2.3.2. This is quite cheap and effective (unless z^{-2} is very close to $[0,1]$), once sufficiently many of the recurrence coefficients for the measure $\mathrm{d}\lambda^{[p]}$ have been precomputed. For $p=2$, $p=3$, the first 100 of them are available to 25 resp. 20 decimal digits in the `OPQ` files `absqm1log1` and `absqm1log2`. They have been computed in quadruple precision by a simplified and extended version of the `ORTHPOLq` routine `qtest2` implementing the procedures discussed in Examples 2.27 and 2.28.

Example 3.70 $R_p(x)$, $p=2$ and 3, and $x = 0.8, 0.9, 0.95, 0.99, 0.999$ and 1.0.

We apply (3.4.30) for $z=x$ in conjunction with the continued fraction algorithm of §2.3.2, using the recurrence coefficients in `absqm1log1` and `absqm1log2`. For the first four values of x we selected `eps0`$= 10^2\times$`eps`, for the others `eps0`$=10^5$ $\times$`eps` resp. `eps0`$=10^{10}\times$`eps`. The `OPQ` routine `Example3_70.m` produces the results shown in Table 3.25. The entries in the second and third column indicate the final starting value[7] of the backward recurrence index ν that yields convergence for the given accuracy tolerance `eps0`. For $x \geq 0.999$, full accuracy could not be achieved with `numax`=100 recurrence coefficients, only the partially accurate results shown in Table 3.25. Interestingly, the continued fraction algorithm seems to converge even for $x=1$, albeit slowly, but there is no theoretical justification for it (to the best of our knowledge).

Table 3.25 *Numerical results for Example 3.70.*

x	$p=2$	$p=3$	$R_2(x)$	$R_3(x)$
0.8	12	11	0.87728809392147	0.82248858052014
0.9	17	15	1.02593895111111	0.93414857586540
0.95	24	21	1.11409957792905	0.99191543992243
0.99	49	40	1.20207566477686	1.03957223187364
0.999	95	57	1.22939819733	1.05056774973
1.000	57	12	1.233625	1.051795

Example 3.71 $R_p(\mathrm{e}^{\mathrm{i}\alpha})$ for $p=2$ and 3, and $\alpha = \omega\pi/2$, $\omega = 0.2, 0.1, 0.05, 0.01, 0.001, 0.000$.

The same procedure as in Example 3.70 was applied, except that the error tolerance for the fifth value of ω was increased to $10^6\times$`eps`. The results, produced by the `OPQ` routine `Example3_71.m`, are shown in Table 3.26. Those for $\mathrm{Re}(R_2)$

[7]The starting value of the recurrence index ν in the routine `cauchy.m` has been increased in steps of 1 rather than 5 to produce the results of Table 3.25.

and $\mathrm{Im}(R_3)$ were checked against the formulae in (3.4.23) and (3.4.24) and found to agree in all but the last digit, which occasionally is off by one unit.

Table 3.26 *Numerical results for Example 3.71.*

p	ω	ν	$\mathrm{Re}(R_p(z))$	$\mathrm{Im}(R_p(z))$
2	0.2	16	0.98696044010894	0.44740227008596
3		15	0.96915102126252	0.34882061265337
2	0.1	21	1.11033049512255	0.27830297928558
3		19	1.02685555765937	0.18409976778928
2	0.05	28	1.17201552262936	0.16639152396897
3		25	1.04449441539672	0.09447224926029
2	0.01	56	1.22136354463481	0.04592009281744
3		47	1.05140829197388	0.01928202831056
2	0.001	97	1.232466849	0.006400460
3		55	1.051794454	0.001936923
2	0.000	57	1.2336	0.0000
3		12	1.0518	0.0000

3.4.5.2 *Series involving ratios of hyperbolic cosine and sine functions* Series of the types

$$T_p(x,b) = \sum_{k=0}^{\infty} \frac{1}{(2k+1)^p} \frac{\cosh(2k+1)x}{\cosh(2k+1)b} \tag{3.4.32}$$

and

$$U_p(x,b) = \sum_{k=0}^{\infty} \frac{1}{(2k+1)^p} \frac{\sinh(2k+1)x}{\cosh(2k+1)b}\,, \tag{3.4.33}$$

where

$$0 \le x \le b, \quad b > 0 \quad \text{and} \quad p = 2, 3, \tag{3.4.34}$$

also are of interest in plate contact problems. They present a more challenging problem of summation, but yield to the procedure of §3.4.5.1 if the ratios of hyperbolic functions are suitably expanded. In the case of (3.4.32), for example, one writes

$$\frac{\cosh(2k+1)x}{\cosh(2k+1)b} = \sum_{n=0}^{\infty} (-1)^n \left\{ \mathrm{e}^{-(2k+1)[(2n+1)b-x]} + \mathrm{e}^{-(2k+1)[(2n+1)b+x]} \right\}$$

and combines this in (3.4.32) with the Laplace transform technique (3.4.26) to obtain (after an elementary calculation using an interchange of the summations over k and n)

$$T_p(x,b) = \frac{1}{2^p(p-1)!} \sum_{n=0}^{\infty} (-1)^n \mathrm{e}^{(2n+1)b} [\varphi_n(-x) + \varphi_n(x)], \tag{3.4.35}$$

where

$$\varphi_n(s) = \mathrm{e}^s \int_0^1 \frac{\mathrm{d}\lambda^{[p]}(t)}{\mathrm{e}^{2[(2n+1)b+s]} - t}, \quad -b \le s \le b, \tag{3.4.36}$$

with $\mathrm{d}\lambda^{[p]}$ as given in (3.4.31). The integral in (3.4.36) is again a Cauchy transform of the measure $\mathrm{d}\lambda^{[p]}$, this time evaluated at $u = \exp(2[(2n+1)b+s])$. Clearly, $u > 1$, unless $n = 0$ and $s = -b$, in which case, by (3.4.30) and (3.4.25),

$$\varphi_0(-b) = \mathrm{e}^{-b} \int_0^1 \frac{\mathrm{d}\lambda^{[p]}(t)}{1-t} = (2^p - 1)(p-1)!\zeta(p)\mathrm{e}^{-b}.$$

The integral in (3.4.36), hence both $\varphi_n(x)$ and $\varphi_n(-x)$ in (3.4.35) (the latter if $n > 0$ or $x < b$), can be computed by the continued fraction algorithm as in §3.4.5.1. For large n, this algorithm converges almost instantaneously. We also note that the series in (3.4.35) converges geometrically with ratio e^{-b}, which is quite satisfactory unless b is small.

For the series (3.4.33) one finds similarly

$$U_p(x,b) = \frac{1}{2^p(p-1)!} \sum_{n=0}^{\infty} (-1)^n \mathrm{e}^{(2n+1)b}[\varphi_n(-x) - \varphi_n(x)], \tag{3.4.37}$$

with convergence behavior similar to the one for the series in (3.4.35). Numerical details can be found in Gautschi (1991c, §5).

Series which include alternating sign factors in (3.4.32) and (3.4.33) can be treated similarly.

3.5 Notes to Chapter 3

§3.1.1. Classical Gauss quadrature formulae (for $\mathrm{d}\lambda(t) = \mathrm{d}t$) have been computed on digital computers as early as 1955; see Davis and Rabinowitz (1956), (1958), who used Newton's method to compute the nodes.

§3.1.1.1. The characterization of the Gauss quadrature nodes as eigenvalues of the Jacobi matrix has been known for some time, among others by physicists, but it is difficult to trace its origin. More recent is the characterization of the Gauss weights in terms of eigenvectors, which was noted in 1962 by Wilf (1978, Chapter 2, Exercise 9) and previously, around 1954, by Goertzel (Wilf, 1980). It has also been used in physics by Gordon (1968). Golub and Welsch (1969) must be credited for having recognized the importance of these characterizations in computing and for having developed a detailed computational procedure based on the QR algorithm.

The eigenvalue/vector characterization of Gauss quadrature rules has become the basis of current methods for computing Gaussian quadrature formulae. This is not to say that they are necessarily the most accurate methods. In special cases, for example Gauss–Legendre formulae, there may well be more efficient and more accurate ways to compute them; for a discussion of this, see Swarztrauber (2002) and the literature cited therein.

Even when adhering to eigenvalue/vector computation, there are alternatives to the Golub–Welsch algorithm based, for example, on rational QR methods or divide-and-conquer algorithms, which may provide better accuracy (Laurie, 2001). In the case of positive definite Jacobi matrices, algorithms based on two-term recursion may also prove to be advantageous; cf. Notes to §1.3 and Laurie (2001).

The remainder term of a Gauss quadrature formula can be estimated either, as in Example 2.47 and Notes to §2.3.3, by contour integration in the complex plane, or by Gauss–Kronrod formulae (§3.1.2.1) or other functionals employing function values on the real line (Ehrich, 2001). The latter technique is frequently used in adaptive quadrature routines.

There is considerable literature on nonpolynomial Gaussian quadrature; see, for example, Gautschi (1981b, §2.3.3). A recent example of interest in dealing with oscillatory integrals is Ixaru and Paternoster (2001); see also Milovanović and Cvetković (2004).

For Gauss quadrature on the unit circle and related Szegö polynomials, see the references cited in the Notes to Chapter 1.

Interval quadrature formulae involve integral averages, rather than point evaluations, of functions in their quadrature sums. The extent to which they can be made "Gaussian" has been discussed by several authors; see Bojanov and Petrov (2001), (2003) and the literature cited therein.

§3.1.1.2. Theorem 3.2 is due to Golub (1973a); the proof given here differs somewhat from the one given in the cited reference. Examples 3.4 and 3.5 are taken from Gautschi (2000a).

§3.1.1.3. Theorem 3.6 is due to Golub (1973a), with the proof given here differing somewhat from the one given in the cited reference. Example 3.8 is from Gautschi (2000b). The numerical problem for very large n, alluded to at the end of this section, was noticed by Velamparambil (1998).

§3.1.1.4. Generalized Gauss–Radau and Gauss–Lobatto formulae with double end points can be found for all four Chebyshev measures in Gautschi and Li (1991).

§3.1.2.1. Soon after Kronrod's work, it has occurred to a number of people, probably first to Patterson (1968), that other quadrature rules can be extended in the manner of Kronrod, for example, Gauss–Radau and Gauss–Lobatto rules. For more recent work on this, see Baratella (1979) and Laurie (2004). Patterson also was the first to consider repeated Kronrod extensions. Starting with a 3-point Gauss–Legendre formula, he was able (numerically) to extend it to a 7-point formula, then extend this formula to a 15-point formula, etc., until reaching a 255-point formula. Rather remarkably, all these extensions have distinct real nodes in $(-1, 1)$ and positive weights; see Patterson (1968), (1973). Gauss–Kronrod extensions for Bernstein–Szegö measures, that is, Chebyshev measures divided by a positive polynomial, are considered in Gautschi and Rivlin (1988), Gautschi and Notaris (1989), and Notaris (1990). Repeated Kronrod extensions of certain interpolatory quadrature rules involving a Bernstein–Szegö

measure are discussed in Peherstorfer (1990b). For Kronrod extensions of generalized Gauss–Radau and Gauss–Lobatto formulae, see Li (1996). A large class of weight functions admitting satisfactory Kronrod extensions for n sufficiently large is identified in Peherstorfer (1990a).

In cases where a satisfactory Kronrod extension does not exist, one may either try to increase the number of Kronrod nodes, as has been done with some success in Kahaner, Waldvogel, and Fullerton (1982), (1984) for the Laguerre measure, or lower the degree of exactness requirement, as has been done in Begumisa and Robinson (1991) for the Hermite measure, among others. An alternative approach, for both these measures, is taken by Ehrich (2002), who suggests using the stratified and anti-Gauss rules of Laurie (1992), (1996) and generalizations thereof. Anti-Gauss rules (see Notes to §1.4.2) rather than Kronrod rules have also been suggested as a means of estimating Gauss quadrature errors; see Laurie (1996). For related work, see also Calvetti and Reichel (2003a).

There are a number of reviews on Gauss–Kronrod quadrature and Stieltjes polynomials; see, for example, Monegato (1979), (1982), (2001), Gautschi (1988), and Notaris (1994). Results on the error of Gauss–Kronrod quadrature formulae are reviewed in Ehrich (1999).

§3.1.2.2. If the Gauss nodes τ_ν are already known, there is a certain redundancy in Laurie's algorithm inasmuch as these Gauss nodes are recomputed along with the Kronrod nodes τ_μ^K. This redundancy is eliminated in an algorithm of Calvetti, Golub, Gragg, and Reichel (2000), which bypasses the computation of the trailing block in (3.1.44) and focuses directly on the Kronrod nodes and the weights of the Gauss–Kronrod formula. Both algorithms assume positivity of the Gauss–Kronrod formula. In the absence of positivity, there are alternative algorithms developed by Ammar, Calvetti, and Reichel (1999).

Most of the earlier work, including Kronrod's, for computing Gauss–Kronrod rules separates the computation of the nodes from that of the weights. Patterson (1968) and Piessens and Branders (1974) expand the Stieltjes polynomial in Legendre resp. Chebyshev polynomials prior to computing its zeros. Monegato (1976), (1978b), Baratella (1979), and Dagnino and Fiorentino (1984) use similar methods to compute π_{n+1}^K for Gegenbauer measures. Kautsky and Elhay (1984) and Elhay and Kautsky (1984) compute the Kronrod nodes as eigenvalues of a certain matrix derived by matrix decomposition methods. A method computing the Kronrod nodes and all weights in one sweep, using Newton's method applied to an appropriate system of nonlinear equations, is discussed in Caliò, Gautschi, and Marchetti (1986). The phenomena noted in the second part of Example 3.19 are new.

§3.1.3.1. Turán's quadrature formula has been generalized by a number of authors to nodes with arbitrary (usually odd) multiplicities, with or without some of the nodes being preassigned. This gives rise to the concept of *σ-orthogonality*, which generalizes s-orthogonality. For surveys of the relevant literature, see Gautschi (1981b, §2.2.2–2.2.4) and Milovanović (2001). For error estimates and constructive methods, see also Milovanović and Spalević (2002). Kronrod ex-

tensions of the Turán formula are considered in Li (1994) and Shi (1996), and generalized Turán–Radau and Turán–Lobatto formulae in Spalević (2002).

There is a large class of measures having the property that all zeros of the corresponding s-orthogonal polynomials are independent of s (Gori and Micchelli, 1996). The respective Gauss–Turán quadrature formulae are useful in evaluating Hilbert transforms and other strongly singular integrals (Cauchy principal value and Hadamard finite part integrals); see, respectively, Gori and Santi (1995) and Gori and Santi (1999).

§3.1.3.2. The basic idea of the method described in this subsection is due to Milovanović (1988). The implementation in Gautschi and Milovanović (1997) uses a slightly different method for computing the weights. In both references, the initial approximations are generated by a discrete homotopy in n (rather than in s, as described here). The method is generalized in Milovanović and Spalević (2002) to σ-orthogonal polynomials and related quadrature rules.

§3.1.4. The original source for quadrature rules of mixed polynomial/rational degree of exactness is Gautschi (1993a), with implementational detail provided later in Gautschi (1999). Another approach, which leads to an eigenvalue/vector characterization similar to the one in §3.1.1.1, has been developed in Bultheel et al. (2003).

There are other ways to deal with poles, especially nearby poles. One is to add a correction term to a standard, in particular Gaussian, quadrature rule. This is an approach taken by Lether, who in Lether (1977b) uses the method of subtracting the singularity, and in Lether (1977a) uses the principal part of the Laurent expansion at each pole to obtain the correction term. The latter, however, requires the evaluation of the regular part of the integrand at each pole. This is avoided in a method proposed by Hunter and Okecha (1986).

§3.1.4.1. Quadrature rules for integrals $\int_{\mathbb{R}} f(t)\,\mathrm{d}\lambda(t)/\omega_m(t)$ and $\mathrm{d}\lambda$ supported on $[-1,1]$ have been studied by López Lagomasino and Illán (1984) from the point of view of convergence, when f is analytic in a domain containing $[-1,1]$ in its interior. They assumed $m = 2n$ and $\zeta_\mu \in (-1,1)$ with $s_\mu = 1$. Theorem 3.25 in this case has been given independently by Van Assche and Vanherwegen (1993, Theorem 1). These authors also consider quadrature rules (3.1.69) with $\operatorname{supp}(\mathrm{d}\lambda) = [-1,1]$ whose nodes are the zeros of the rational function $(1+\zeta_n t)^{-1} + \sum_{\mu=1}^{n-1} c_\mu (1+\zeta_\mu t)^{-1}$ orthogonal (in the measure $\mathrm{d}\lambda$) to 1 and to $(1+\zeta_\nu t)^{-1}$, $\nu = 1, 2, \ldots, n-1$. Although no longer "Gaussian" rules, they require for their construction polynomials orthogonal with respect to the measure $\mathrm{d}\lambda/\omega_{n-1}\omega_n$. The use of conjugate complex parameters ζ_μ is considered in López Lagomasino and Illán González (1987). Theorem 3.25 in the general form stated here is from Gautschi (1993a), and so are the Examples 3.31–3.32.

The implementation of Theorem 3.25 given here is based on the discrete Stieltjes procedure, which enjoys general applicability. Alternatively, one could try to use the modified Chebyshev algorithm with modified moments defined by $m_k = \int_{\mathbb{R}} p_k(t)\,\mathrm{d}\lambda(t)/\omega_m(t)$. The major difficulty with this is the accurate computation of the moments. This is true even in the simple case of $\mathrm{d}\lambda(t) = \mathrm{d}t$ on

$[-1, 1]$ and $p_k = T_k$ the Chebyshev polynomials, which, however, was successfully resolved in Weideman and Laurie (2000) by a skillful use of recurrence relations. The same authors also develop rational Fejér quadrature rules.

Rational Gauss formulae for the Chebyshev measure and real poles of multiplicity 2, with the space $\mathbb{S}_{2n} = \mathbb{Q}_{2n}$ being purely rational, are studied in Min (1998a).

§3.1.4.2. The procedures developed here for treating difficult poles were proposed in Gautschi (1999, §3.4).

§3.1.4.3. The application of rational Gauss formulae to generalized Fermi–Dirac and Bose–Einstein integrals is further discussed in Gautschi (1993c). The modification suggested for large θ is from Gautschi (1999, §5).

§3.1.4.4. The material in this subsection is new. Rational Gauss–Lobatto quadrature rules for the Chebyshev measure, however, have been studied by Min (1998b).

§3.1.4.5–3.1.4.6. This follows closely the treatment in Gautschi, Gori, and Lo Cascio (2000).

§3.1.5. Quadrature formulae for Cauchy principal value integrals, especially the elegant formula (3.1.123), but also the numerical implementations in §3.1.5.3, are due to Korneĭčuk (1964). Many of these formulae have been rediscovered later on by other authors. For references, see Gautschi (1981b, §3.2).

§3.1.5.3. Another way of circumventing the loss of accuracy when x is near a Gauss node τ_ν^G is to evaluate $\mathcal{C}f(x; \mathrm{d}\lambda)$ by either (3.1.121) or (3.1.125) at the nodes of the $(n + 1)$-point Gauss formula and then use polynomial (or other) interpolation to evaluate $\mathcal{C}f(x; \mathrm{d}\lambda)$ for arbitrary x. This was proposed by Diethelm (1999) and implemented for the Hermite measure $\mathrm{d}\lambda(t) = \exp(-t^2)\,\mathrm{d}t$ on $\mathbb{R}$. Similar methods for the Hermite and Laguerre measures are discussed, respectively, in De Bonis, Della Vecchia, and Mastroianni (2002a) and De Bonis, Della Vecchia, and Mastroianni (2002b); see also Capobianco, Criscuolo, and Giova (2001).

§3.1.6. The techniques discussed in this section, the one based on Stieltjes's procedure and the one based on the modified Chebyshev algorithm, and especially also the matrix formulation of Gauss quadrature sums used in these techniques, are due to Fischer and Golub (1991). Example 3.45 is new.

§3.1.7. Solutions to the problem of estimating matrix functionals of the type considered have many applications, besides those mentioned in §3.1.7.2. See, for example, Golub and von Matt (1991) for applications to constrained matrix least squares problems, and Calvetti, Hansen, and Reichel (2002), Calvetti and Reichel (2003b) (also Hanke (2003)) for applications to the evaluation of regularization parameters in Tikhonov regularization. The case $f(t) = (\lambda - t)^{-1}$ with λ outside the spectrum of $\boldsymbol{A}$ has important applications in physical chemistry and solid state physics; see Golub and Strakoš (1994, §1) for references.

The use of orthogonal polynomials for discrete measures supported on the spectrum of positive definite matrices has been pioneered by Hestenes and Stiefel (1952) and Stiefel (1958).

Calvetti, Reichel, and Sgallari (1999) use anti-Gauss quadrature rules (see Notes to §1.4.2) instead of Gauss–Radau and Gauss–Lobatto rules for estimating matrix functionals.

§3.1.7.1. The original source for the Lanczos algorithm is Lanczos (1950). Some of the uses of this algorithm in numerical linear algebra are reviewed in Golub (1973b).

§3.1.7.2. The use of quadrature methods in obtaining error bounds for the solution of linear algebraic systems goes back to Dahlquist, Eisenstat, and Golub (1972). The results for estimating diagonal elements of the inverse of a positive definite matrix are from Golub and Meurant (1994, Theorem 5.1).

§3.2.1. Much of the material in this subsection is well established. The device in (3.2.10) of improving the accuracy, and the related Algorithm 3.4, are due to de Boor (Conte and de Boor, 1972, §4.11). The approximations discussed in Examples 3.49 and 3.50 can be found in many texts on Chebyshev polynomials, for example, Fox and Parker (1968, §2.13) and Mason and Handscomb (2003, §6.3).

Equation (3.2.6) shows that least squares approximation is "moment-preserving" in terms of modified moments (cf. §3.3). For extensions of this observation, see Bojanov and Gori (1999).

The sensitivity of the coefficients in the least squares solution to small perturbations in the data is studied in Beckermann and Saff (1999).

In real-time applications it is often required to process a stream of continuously arriving data and to update and downdate least squares approximations relative to moving "time windows." For a discussion of this, see Elhay, Golub, and Kautsky (1991) and Fuchs (1999).

§3.2.2. The reduction of constrained least squares problems to unconstrained ones is part of folklore; an explicit mention thereof can be found in Gautschi (1989, §8). Examples 3.51 and 3.52 are new.

§3.2.3. For the history of this problem, see the Notes to §1.7. Algorithm 3.5 is new in the context of Sobolev least squares approximation, and so is Example 3.53.

§3.3.1. The connection between moment-preserving spline approximation and Gaussian quadrature was first observed by Gautschi (1984a) in the context of piecewise constant, and Dirac delta function, approximation. The extension to spline functions of arbitrary degree was carried out in Gautschi and Milovanović (1986b); for a summary, see also Gautschi (1992). Moment-preserving approximation by defective splines is related to generalized Gauss–Turán quadrature; for this, see Milovanović and Kovačević (1988), Kovačević and Milovanović (1996), Gori N. Amati and Santi (1990), and Milovanović (2001, §5).

§3.3.2. Further extensions of the approximation problem on $[0, 1]$ are discussed by Micchelli (1988), who relates moment-preserving approximation to the theory of monosplines. A similar approach is taken by Gori and Santi (1992) to deal with defective splines. For these, see also Frontini and Milovanović (1989).

§3.4.1. The summation procedure described in this subsection was first suggested in Gautschi and Milovanović (1985). It was implemented using Gauss–Einstein and Gauss–Fermi quadratures. The alternative use of rational Gauss–Laguerre formulae, although mentioned in Gautschi (1996, §3.2), is implemented here for the first time. The series of Example 3.63 is a special case of the series $\sum k^{\nu-1} r(k)$, where $0 < \nu \leq 1$ and r is a rational function. Summation of these more general series and their alternating companion series is discussed in Gautschi (1991a). An alternative approach, using Euler–Maclaurin summation, is considered in Lewanowicz (1994b). For the Hardy–Littlewood function $H(x)$, see Gautschi (2004), where a more effective summation procedure is proposed that works also for large values of x.

§3.4.2–3.4.4. The material in these subsections is taken from Gautschi and Milovanović (1985).

§3.4.5. This section follows Gautschi (1991c). See also Boersma and Dempsey (1992) for alternative methods.

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Bibliography

Abramowitz, M. and I. A. Stegun (1992). *Handbook of mathematical functions with formulas, graphs, and mathematical tables*. New York: Dover Publications, Inc. Reprint of the 1972 edition.

Althammer, P. (1962). Eine Erweiterung des Orthogonalitätsbegriffes bei Polynomen und deren Anwendung auf die beste Approximation. *J. Reine Angew. Math. 211*(3–4), 192–204.

Alzer, H., C. Berg, and S. Koumandos (2004). On a conjecture of Clark and Ismail. *J. Approx. Theory*, to appear.

Ammar, G. S., W. B. Gragg, and L. Reichel (1993). An analogue for Szegö polynomials of the Clenshaw algorithm. Computational complex analysis. *J. Comput. Appl. Math. 46*(1–2), 211–216.

Ammar, G. S., D. Calvetti, and L. Reichel (1999). Computation of Gauss–Kronrod quadrature rules with non-positive weights. Orthogonal polynomials: numerical and symbolic algorithms (Leganés, 1998). *Electron. Trans. Numer. Anal. 9*, 26–38 (electronic).

Aptekarev, A. I. (1998). Multiple orthogonal polynomials. Proceedings of the VIIIth Symposium on Orthogonal Polynomials and their Applications (Seville, 1997). *J. Comput. Appl. Math. 99*(1–2), 423–447.

Aptekarev, A. I., A. Branquinho, and W. Van Assche (2003). Multiple orthogonal polynomials for classical weights. *Trans. Amer. Math. Soc 355*(10), 3887–3914. electronic.

Arvesú, J., J. Coussement, and W. Van Assche (2003). Some discrete multiple orthogonal polynomials. Proceedings of the Sixth International Symposium on Orthogonal Polynomials, Special Functions and their Applications (Rome, 2001). *J. Comput. Appl. Math 153*(1–2), 19–45.

Askey, R. and J. Wilson (1985). Some basic hypergeometric orthogonal polynomials that generalize Jacobi polynomials. *Mem. Amer. Math. Soc. 54*(319), iv+55.

Baillaud, B. and H. Bourget (1905). *Correspondance d'Hermite et de Stieltjes*, Volumes I and II. Paris: Gauthier-Villars. Avec une préface de Émile Picard.

Ball, J. S. (2003). Half-range generalized Hermite polynomials and the related Gaussian quadratures. *SIAM J. Numer. Anal. 40*(6), 2311–2317.

Bannai, E. (1990). Orthogonal polynomials in coding theory and algebraic combinatorics. In P. Nevai (Ed.), *Orthogonal polynomials (Columbus, OH, 1989)*, Volume 294 of *NATO Adv. Sci. Inst. Ser. C Math. Phys. Sci.*, pp. 25–53. Dordrecht: Kluwer.

Baratella, P. (1979). Un'estensione ottimale della fomula di quadratura di Radau. *Rend. Sem. Mat. Univ. Politec. Torino 37*(1), 147–158.

Barkov, G. I. (1960). Some systems of polynomials orthogonal in two symmetric intervals. *Izv. Vyssˇ. Učebn. Zav. Matematika No. 4*, 3–16. Russian.

Barrio, R. (2000). Parallel algorithms to evaluate orthogonal polynomial series. *SIAM J. Sci. Comput. 21*(6), 2225–2239.

Barrio, R. (2002). Rounding error bounds for the Clenshaw and Forsythe algorithms for the evaluation of orthogonal polynomial series. *J. Comput. Appl. Math. 138*(2), 185–204.

Beckermann, B. (2001). Complex Jacobi matrices. Numerical analysis 2000, Vol. 5, Quadrature and orthogonal polynomials. *J. Comput. Appl. Math. 127*(1–2), 17–65.

Beckermann, B. and E. Bourreau (1998). How to choose modified moments? *J. Comput. Appl. Math. 98*(1), 81–98.

Beckermann, B. and E. B. Saff (1999). The sensitivity of least squares polynomial approximation. In W. Gautschi, G. H. Golub, and G. Opfer (Eds), *Applications and computation of orthogonal polynomials (Oberwolfach, 1998)*, Volume 131 of *International Series of Numerical Mathematics*, pp. 1–19. Basel: Birkhäuser.

Beckermann, B., J. Coussement, and W. Van Assche (2004). Multiple Wilson and Jacobi–Piñeiro polynomials. Submitted for publication.

Begumisa, A. and I. Robinson (1991). Suboptimal Kronrod extension formulae for numerical quadrature. *Numer. Math. 58*(8), 807–818.

Bernstein, S. (1930). Sur les polynomes orthogonaux relatifs à un segment fini. *J. Math. Pures Appl. (9) 9*, 127–177.

Berti, A. C. and A. Sri Ranga (2001). Companion orthogonal polynomials: some applications. *Appl. Numer. Math. 39*(2), 127–149.

Blue, J. L. (1979). A Legendre polynomial integral. *Math. Comp. 33*(146), 739–741.

Boersma, J. and J. P. Dempsey (1992). On the numerical evaluation of Legendre's chi-function. *Math. Comp. 59*(199), 157–163.

Bojanov, B. and L. Gori (1999). Moment-preserving approximations. *Math. Balkanica (N.S.) 13*(3–4), 385–398.

Bojanov, B. D. and P. P. Petrov (2001). Gaussian interval quadrature formula. *Numer. Math. 87*(4), 625–643.

Bojanov, B. and P. Petrov (2003). Uniqueness of the Gaussian interval quadrature formula. *Numer. Math. 95*(1), 53–62.

Borges, C. F. (1994). On a class of Gauss-like quadrature rules. *Numer. Math. 67*(3), 271–288.

Bourreau, E. (2000). Modified moments and matrix orthogonal polynomials. Proceedings of the International Conference on Rational Approximation, ICRA99 (Antwerp). *Acta Appl. Math. 61*(1–3), 53–64.

Brenner, J. (1969). *Über eine Erweiterung des Orthogonalitätsbegriffes bei Polynomen in einer und zwei Variablen*. Ph.D. thesis, Universität Stuttgart (Technische Hochschule), Stuttgart.

Brezinski, C. and M. Redivo Zaglia (1991). *Extrapolation methods. Theory and practice*, Volume 2 of *Studies in Computational Mathematics*. Amsterdam: North-Holland Publishing Co. With 1 IBM-PC floppy disk (5.25 inch).

British Association for the Advancement of Science (1952). *Mathematical tables, Volume 10, Bessel functions, Part II, Functions of positive integer order*. Cambrige: Cambridge Univ. Press.

Bultheel, A. and M. Van Barel (1997). *Linear algebra, rational approximation and orthogonal polynomials*, Volume 6 of *Studies in Computational Mathematics*. Amsterdam: North-Holland Publishing Co.

Bultheel, A., P. González-Vera, E. Hendriksen, and O. Njåstad (1994). Numerical quadratures on the unit circle. A survey with some new results. In M. Alfaro, A. García, C. Jagels, and F. Marcellán (Eds), *Orthogonal polynomials on the unit circle: theory and applications (Madrid, 1994)*, Leganés, pp. 1–20. University Carlos III Madrid.

Bultheel, A., L. Daruis, and P. González-Vera (2001). A connection between quadrature formulas on the unit circle and the interval $[-1, 1]$. Advanced numerical methods for mathematical modelling. *J. Comput. Appl. Math. 132*(1), 1–14.

Bultheel, A., P. González-Vera, E. Hendriksen, and O. Njåstad (2001). Quadrature and orthogonal rational functions. Numerical analysis 2000, Vol. 5, Quadrature and orthogonal polynomials. *J. Comput. Appl. Math. 127*(1–2), 67–91.

Bultheel, A., P. González-Vera, E. Hendriksen, and O. Njåstad (2003). Orthogonal rational functions and tridiagonal matrices. Proceedings of the Sixth International Symposium on Orthogonal Polynomials, Special Functions and their Applications (Rome, 2001). *J. Comput. Appl. Math. 153*(1–2), 89–97.

Calder, A. C. and J. G. Laframboise (1986). Multiple-water-bag simulation of inhomogeneous plasma motion near an electrode. *J. Comput. Phys. 65*(1), 18–45.

Caliò, F., W. Gautschi, and E. Marchetti (1986). On computing Gauss–Kronrod quadrature formulae. *Math. Comp. 47*(176), 639–650. Supplement, *ibid.*, pp. S57–S63.

Calvetti, D. and L. Reichel (2003a). Symmetric Gauss-Lobatto and modified anti-Gauss rules. *BIT Numer. Math. 43*(3), 541–554.

Calvetti, D. and L. Reichel (2003b). Tikhonov regularization of large problems. *BIT Numer. Math. 43*(2), 263–283.

Calvetti, D., L. Reichel, and F. Sgallari (1999). Applications of anti-Gauss quadrature rules in linear algebra. In W. Gautschi, G. H. Golub, and G. Opfer

(Eds), *Applications and computation of orthogonal polynomials (Oberwolfach, 1998)*, Volume 131 of *Internat. Ser. Numer. Math.*, pp. 41–56. Basel: Birkhäuser.

Calvetti, D., G. H. Golub, W. B. Gragg, and L. Reichel (2000). Computation of Gauss–Kronrod rules. *Math. Comp. 69*(231), 1035–1052.

Calvetti, D., P. C. Hansen, and L. Reichel (2002). L-curve curvature bounds via Lanczos bidiagonalization. Orthogonal polynomials, approximation theory, and harmonic analysis (Inzel, 2000). *Electron. Trans. Numer. Anal. 14*, 20–35 (electronic).

Capobianco, M. R., G. Criscuolo, and R. Giova (2001). A stable and convergent algorithm to evaluate Hilbert transform. In memory of W. Gross. *Numer. Algorithms 28*(1–4), 11–26.

Chebyshev, P. L. (1859). Sur l'interpolation par la méthode des moindres carrés. *Mém. Acad. Impér. Sci. St. Petersbourg (7) 1*(15), 1–24. Also in *Œuvres I*, pp. 473–498.

Cheng, H., V. Rokhlin, and N. Yarvin (1999). Nonlinear optimization, quadrature, and interpolation. *SIAM J. Optim. 9*(4), 901–923 (electronic).

Chihara, T. S. (1978). *An introduction to orthogonal polynomials*, Volume 13 of *Mathematics and its Applications*. New York: Gordon and Breach Science Publishers.

Chihara, T. S. (1985). Orthogonal polynomials and measures with end point masses. *Rocky Mountain J. Math. 15*(3), 705–719.

Chin, R. C. Y. (1992). A domain decomposition method for generating orthogonal polynomials for a Gaussian weight on a finite interval. *J. Comput. Phys. 99*(2), 321–336.

Chinellato, O. (2003). Personal communication.

Christoffel, E. B. (1858). Über die Gaußische Quadratur und eine Verallgemeinerung derselben. *J. Reine Angew. Math. 55*, 61–82. Also in *Ges. Math. Abhandlungen I*, pp. 42–50.

Christoffel, E. B. (1877). Sur une classe particulière de fonctions entières et de fractions continues. *Ann. Mat. Pura Appl. 8*, 1–10. Also in *Ges. Math. Abhandlungen II*, pp. 42–50.

Clark, W. E. and M. E. H. Ismail (2003). Inequalities involving gamma and psi functions. *Anal. Appl. 1*(1), 129–140.

Clenshaw, C. W. (1955). A note on the summation of Chebyshev series. *Math. Tables Aids Comput. 9*(51), 118–120.

Cohen, Jr., E. A. (1975). Zero distribution and behavior of orthogonal polynomials in the Sobolev space $W^{1,2}[-1,1]$. *SIAM J. Math. Anal. 6*(1), 105–116.

Conte, S. D. and C. de Boor (1972). *Elementary numerical analysis: an algorithmic approach* (2nd edn). *International Series in Pure and Applied Mathematics*. New York: McGraw-Hill Book Company.

Cooper, G. J. (1967). The evaluation of the coefficients in a Chebyshev expansion. *Comput. J. 10*(1), 94–100.

Coussement, E. and W. Van Assche (2003). Multiple orthogonal polynomials associated with the modified Bessel functions of the first kind. *Constr. Approx. 19*(2), 237–263.

Dagnino, C. and C. Fiorentino (1984). Computation of nodes and weights of extended Gaussian rules. *Computing 32*(3), 271–278.

Dahlquist, G., S. C. Eisenstat, and G. H. Golub (1972). Bounds for the error of linear systems of equations using the theory of moments. *J. Math. Anal. Appl. 37*(1), 151–166.

Daruis, L. and P. González-Vera (2001). Szegö polynomials and quadrature formulas on the unit circle. *Appl. Numer. Math. 36*(1), 79–112.

Daruis, L., P. González-Vera, and O. Njåstad (2001). Szegö quadrature formulas for certain Jacobi-type weight functions. *Math. Comp. 71*(238), 683–701.

Davis, P. J. (1975). *Interpolation and approximation*. New York: Dover Publications, Inc. Republication, with minor corrections, of the 1963 original, with a new preface and bibliography.

Davis, P. J. (1993). *Spirals: from Theodorus to chaos*. Wellesley, MA: A K Peters, Ltd. With contributions by Walter Gautschi and Arieh Iserles.

Davis, P. and P. Rabinowitz (1956). Abscissas and weights for Gaussian quadratures of high order. *J. Res. Nat. Bur. Standards 56*(1), 35–37.

Davis, P. and P. Rabinowitz (1958). Additional abscissas and weights for Gaussian quadratures of high order. Values for $n = 64$, 80, and 96. *J. Res. Nat. Bur. Standards 60*(6), 613–614.

Davis, P. J. and P. Rabinowitz (1984). *Methods of numerical integration* (2nd edn). Computer Science and Applied Mathematics. Orlando, FL: Academic Press Inc.

De Bonis, M. C., B. Della Vecchia, and G. Mastroianni (2002a). Approximation of the Hilbert transform on the real line using Hermite zeros. *Math. Comp. 71*(239), 1169–1188.

De Bonis, M. C., B. Della Vecchia, and G. Mastroianni (2002b). Approximation of the Hilbert transform on the real semiaxis using Laguerre zeros. Proceedings of the 9th International Congress on Computational and Applied Mathematics (Leuven, 2000). *J. Comput. Appl. Math. 140*(1–2), 209–229.

de Bruin, M. G. (1990). Polynomials orthogonal on a circular arc. *J. Comput. Appl. Math. 31*(2), 253–266.

Deift, P. A. (1999). *Orthogonal polynomials and random matrices: a Riemann–Hilbert approach*, Volume 3 of *Courant Lecture Notes in Math.* New York: Courant Institute of Mathematical Sciences, New York University.

Delahaye, J.-P. (1988). *Sequence transformations*, Volume 11 of *Springer Series in Computational Mathematics*. Berlin: Springer-Verlag. With an introduction by Claude Brezinski.

Deuflhard, P. (1974). On algorithms for the summation of certain special functions. Bericht 7407, Techn. Univ. München, Abteilung Mathematik, München.

Deuflhard, P. (1977). A summation technique for minimal solutions of linear homogeneous difference equations. *Computing 18*(1), 1–13.

Diethelm, K. (1999). A method for the practical evaluation of the Hilbert transform on the real line. Numerical evaluation of integrals. *J. Comput. Appl. Math. 112*(1–2), 45–53.

Driscoll, T. A. and L. N. Trefethen (2002). *Schwarz–Christoffel mapping*, Volume 8 of *Cambridge Monographs on Applied and Computational Mathematics*. Cambridge: Cambridge Univ. Press.

Dunkl, C. F. and Y. Xu (2001). *Orthogonal polynomials of several variables*, Volume 81 of *Encyclopedia of Mathematics and its Applications*. Cambridge: Cambridge Univ. Press.

Durán, A. J. and E. Defez (2002). Orthogonal matrix polynomials and quadrature formulas. *Linear Algebra Appl. 345*, 71–84.

Durán, A. J. and B. Polo (2002). Gaussian quadrature formulae for matrix weights. *Linear Algebra Appl. 355*, 119–146.

Ehrich, S. (1999). Stieltjes polynomials and the error of Gauss–Kronrod quadrature formulas. In W. Gautschi, G. H. Golub, and G. Opfer (Eds), *Applications and computation of orthogonal polynomials (Oberwolfach, 1998)*, Volume 131 of *Internat. Ser. Numer. Math.*, pp. 57–77. Basel: Birkhäuser.

Ehrich, S. (2001). Stopping functionals for Gaussian quadrature formulas. Numerical analysis 2000, Vol. 5, Quadrature and orthogonal polynomials. *J. Comput. Appl. Math. 127*(1–2), 153–171.

Ehrich, S. (2002). On stratified extensions of Gauss–Laguerre and Gauss–Hermite quadrature formulas. Proceedings of the 9th International Congress on Computational and Applied Mathematics (Leuven, 2000). *J. Comput. Appl. Math. 140*(1–2), 291–299.

Elhay, S. and J. Kautsky (1984). A method for computing quadratures of the Kronrod Patterson type. *Austral. Comput. Sci. Comm. 6*(1), 15.1–15.9.

Elhay, S., G. H. Golub, and J. Kautsky (1991). Updating and downdating of orthogonal polynomials with data fitting applications. *SIAM J. Matrix Anal. Appl. 12*(2), 327–353.

Elliott, D. (1968). Error analysis of an algorithm for summing certain finite series. *J. Austral. Math. Society 8*(2), 213–221.

Erdélyi, A., W. Magnus, F. Oberhettinger, and F. G. Tricomi (1954). *Tables of integral transforms*, Volume II. New York: McGraw-Hill Book Company, Inc. Based, in part, on notes left by Harry Bateman.

Evans, W. D., L. L. Littlejohn, F. Marcellán, C. Markett, and A. Ronveaux (1995). On recurrence relations for Sobolev orthogonal polynomials. *SIAM J. Math. Anal. 26*(2), 446–467.

Fejér, L. (1933). Mechanische Quadraturen mit positiven Cotesschen Zahlen. *Math. Z. 37*, 287–309. Also in *Ges. Arbeiten II*, pp. 457–478.

Fischer, B. and G. H. Golub (1991). On generating polynomials which are orthogonal over several intervals. *Math. Comp. 56*(194), 711–730.

Fischer, B. and G. H. Golub (1992). How to generate unknown orthogonal polynomials out of known orthogonal polynomials. Orthogonal polynomials and numerical methods. *J. Comput. Appl. Math. 43*(1–2), 99–115.

Fischer, H.-J. (1996). On the condition of orthogonal polynomials via modified moments. *Z. Anal. Anwendungen 15*(1), 223–244.

Fischer, H.-J. (1998). Explicit calculation of some polynomials introduced by W. Gautschi. *Z. Anal. Anwendungen 17*(4), 963–977.

Forsythe, G. E. (1957). Generation and use of orthogonal polynomials for data-fitting with a digital computer. *J. Soc. Indust. Appl. Math. 5*(2), 74–88.

Fox, L. and I. Parker (1968). *Chebyshev polynomials in numerical analysis*. London: Oxford Univ. Press.

Freud, G. (1971). *Orthogonal polynomials*. New York: Pergamon Press, Inc. English translation of *Orthogonale Polynome*. Basel: Birkhäuser, 1969.

Freund, R. W. (2001). Computation of matrix-valued formally orthogonal polynomials and applications. Numerical analysis 2000, Vol. 5, Quadrature and orthogonal polynomials. *J. Comput. Appl. Math. 127*(1–2), 173–199.

Frontini, M. and G. V. Milovanović (1989). Moment-preserving spline approximation on finite intervals and Turán quadratures. *Facta Univ. Ser. Math. Inform. No. 4*, 45–56.

Frontini, M., W. Gautschi, and G. V. Milovanović (1987). Moment-preserving spline approximation on finite intervals. *Numer. Math. 50*(5), 503–518.

Fuchs, E. (1999). On discrete polynomial least-squares approximation in moving time windows. In W. Gautschi, G. H. Golub, and G. Opfer (Eds), *Applications and computation of orthogonal polynomials (Oberwolfach, 1998)*, Volume 131 of *International Series of Numerical Mathematics*, pp. 93–107. Basel: Birkhäuser.

Gakhov, F. D. (1990). *Boundary value problems*. New York: Dover Publications, Inc. Translated from the Russian. Reprint of the 1966 translation.

Galant, D. (1971). An implementation of Christoffel's theorem in the theory of orthogonal polynomials. *Math. Comp. 25*(113), 111–113.

Gatteschi, L. (1964). Su una formula di quadratura "quasi gaussiana". Tabulazione delle ascisse d'integrazione e delle relative costanti di Christoffel. *Atti Accad. Sci. Torino Cl. Sci. Fis. Mat. Natur. 98*(5), 641–661.

Gatteschi, L. (1980). On some orthogonal polynomial integrals. *Math. Comp. 35*(152), 1291–1298.

Gauss, C. F. (1814). Methodus nova integralium valores per approximationem inveniendi. *Commentationes Societatis Regiae Scientarium Gottingensis Recentiores 3*. Also in *Werke III*, pp. 163–196.

Gautschi, W. (1963). On inverses of Vandermonde and confluent Vandermonde matrices. II. *Numer. Math. 5*(5), 425–430.

Gautschi, W. (1967a). Computational aspects of three-term recurrence relations. *SIAM Rev. 9*(1), 24–82.

Gautschi, W. (1967b). Numerical quadrature in the presence of a singularity. *SIAM J. Numer. Anal. 4*(3), 357–362.

Gautschi, W. (1968). Construction of Gauss–Christoffel quadrature formulas. *Math. Comp. 22*(102), 251–270.

Gautschi, W. (1970). On the construction of Gaussian quadrature rules from modified moments. *Math. Comp. 24*(110), 245–260.

Gautschi, W. (1979). On the preceding paper "A Legendre polynomial integral" by James L. Blue. *Math. Comp. 33*(146), 742–743.

Gautschi, W. (1981a). Minimal solutions of three-term recurrence relations and orthogonal polynomials. *Math. Comp. 36*(154), 547–554.

Gautschi, W. (1981b). A survey of Gauss–Christoffel quadrature formulae. In P. L. Butzer and F. Fehér (Eds), *E. B. Christoffel (Aachen/Monschau, 1979)*, pp. 72–147. Basel: Birkhäuser.

Gautschi, W. (1982a). An algorithmic implementation of the generalized Christoffel theorem. In G. Hämmerlin (Ed.), *Numerical integration*, Volume 57 of *Internat. Ser. Numer. Math.*, pp. 89–106. Basel: Birkhäuser.

Gautschi, W. (1982b). On generating orthogonal polynomials. *SIAM J. Sci. Statist. Comput. 3*(3), 289–317.

Gautschi, W. (1983). How and how not to check Gaussian quadrature formulae. *BIT 23*(2), 209–216.

Gautschi, W. (1984a). Discrete approximations to spherically symmetric distributions. *Numer. Math. 44*(1), 53–60.

Gautschi, W. (1984b). On some orthogonal polynomials of interest in theoretical chemistry. *BIT 24*(4), 473–483.

Gautschi, W. (1984c). Questions of numerical condition related to polynomials. In G. H. Golub (Ed.), *Studies in numerical analysis*, Volume 24 of *MAA Stud. Math.*, pp. 140–177. Washington, DC: Math. Assoc. America.

Gautschi, W. (1986). On the sensitivity of orthogonal polynomials to perturbations in the moments. *Numer. Math. 48*(4), 369–382.

Gautschi, W. (1988). Gauss–Kronrod quadrature—a survey. In *Numerical methods and approximation III (Niš, 1987)*, pp. 39–66. Niš: Univ. Niš.

Gautschi, W. (1989). Orthogonality—conventional and unconventional—in numerical analysis. In K. Bowers and J. Lund (Eds), *Computation and control (Bozeman, MT, 1988)*, Volume 1 of *Progr. Systems Control Theory*, pp. 63–95. Boston, MA: Birkhäuser Boston.

Gautschi, W. (1990). Computational aspects of orthogonal polynomials. In P. Nevai (Ed.), *Orthogonal polynomials (Columbus, OH, 1989)*, Volume 294 of *NATO Adv. Sci. Inst. Ser. C Math. Phys. Sci.*, pp. 181–216. Dordrecht: Kluwer.

Gautschi, W. (1991a). A class of slowly convergent series and their summation by Gaussian quadrature. *Math. Comp. 57*(195), 309–324.

Gautschi, W. (1991b). Computational problems and applications of orthogonal polynomials. In C. Brezinski, L. Gori, and A. Ronveaux (Eds), *Orthogonal polynomials and their applications (Erice, 1990)*, Volume 9 of *IMACS Ann. Comput. Appl. Math.*, pp. 63–95. Basel: Baltzer.

Gautschi, W. (1991c). On certain slowly convergent series occurring in plate contact problems. *Math. Comp. 57*(195), 325–338.

Gautschi, W. (1991d). On the remainder term for analytic functions of Gauss–Lobatto and Gauss–Radau quadratures. Proceedings of the U.S.–Western Europe Regional Conference on Padé Approximants and Related Topics (Boulder, CO, 1988). *Rocky Mountain J. Math. 21*(1), 209–226. Corrections, *ibid. 21*(3) (1991), p. 1143.

Gautschi, W. (1992). Spline approximation and quadrature formulae. *Atti Sem. Mat. Fis. Univ. Modena 40*(1), 169–182.

Gautschi, W. (1993a). Gauss-type quadrature rules for rational functions. In H. Brass and G. Hämmerlin (Eds), *Numerical integration, IV (Oberwolfach, 1992)*, Volume 112 of *Internat. Ser. Numer. Math.*, pp. 111–130. Basel: Birkhäuser.

Gautschi, W. (1993b). Is the recurrence relation for orthogonal polynomials always stable? *BIT 33*(2), 277–284.

Gautschi, W. (1993c). On the computation of generalized Fermi–Dirac and Bose–Einstein integrals. *Comput. Phys. Comm. 74*(2), 233–238.

Gautschi, W. (1994). Algorithm 726—ORTHPOL: a package of routines for generating orthogonal polynomials and Gauss-type quadrature rules. *ACM Trans. Math. Software 20*(1), 21–62.

Gautschi, W. (1996). Orthogonal polynomials: applications and computation. In A. Iserles (Ed.), *Acta Numerica, 1996*, Volume 5 of *Acta Numerica*, pp. 45–119. Cambridge: Cambridge Univ. Press.

Gautschi, W. (1997a). The computation of special functions by linear difference equations. In S. Elaydi, I. Győri, and G. Ladas (Eds), *Advances in difference equations (Veszprém, 1995)*, pp. 213–243. Amsterdam: Gordon and Breach.

Gautschi, W. (1997b). *Numerical analysis. An introduction.* Boston, MA: Birkhäuser Boston Inc.

Gautschi, W. (1997c). On the computation of special Sobolev-type orthogonal polynomials. The heritage of P. L. Chebyshev: a Festschrift in honor of the 70th birthday of T. J. Rivlin. *Ann. Numer. Math. 4*(1–4), 329–342.

Gautschi, W. (1999). Algorithm 793: GQRAT—Gauss quadrature for rational functions. *ACM Trans. Math. Software 25*(2), 213–239.

Gautschi, W. (2000a). Gauss–Radau formulae for Jacobi and Laguerre weight functions. 1999 International Symposium on Computational Sciences, to honor John R. Rice (West Lafayette, IN). *Math. Comput. Simulation 54*(4–5), 403–412.

Gautschi, W. (2000b). High-order Gauss–Lobatto formulae. Mathematical journey through analysis, matrix theory and scientific computation (Kent, OH, 1999). *Numer. Algorithms 25*(1–4), 213–222.

Gautschi, W. (2002). The interplay between classical analysis and (numerical) linear algebra—a tribute to Gene H. Golub. *Electron. Trans. Numer. Anal. 13*, 119–147 (electronic).

Gautschi, W. (2004). The Hardy–Littlewood function: an exercise in slowly convergent series. *J. Comput. Appl. Math.*, to appear.

Gautschi, W. and S. Li (1990). The remainder term for analytic functions of Gauss–Radau and Gauss–Lobatto quadrature rules with multiple end points. *J. Comput. Appl. Math. 33*(3), 315–329.

Gautschi, W. and S. Li (1991). Gauss–Radau and Gauss–Lobatto quadratures with double end points. *J. Comput. Appl. Math. 34*(3), 343–360.

Gautschi, W. and S. Li (1993). A set of orthogonal polynomials induced by a given orthogonal polynomial. *Aequationes Math. 46*(1–2), 174–198.

Gautschi, W. and G. V. Milovanović (1985). Gaussian quadrature involving Einstein and Fermi functions with an application to summation of series. *Math. Comp. 44*(169), 177–190.

Gautschi, W. and G. V. Milovanović (1986a). Polynomials orthogonal on the semicircle. *J. Approx. Theory 46*(3), 230–250.

Gautschi, W. and G. V. Milovanović (1986b). Spline approximations to spherically symmetric distributions. *Numer. Math. 49*(2–3), 111–121.

Gautschi, W. and G. V. Milovanović (1997). s-orthogonality and construction of Gauss–Turán-type quadrature formulae. Special issue dedicated to William B. Gragg (Monterey, CA, 1996). *J. Comput. Appl. Math. 86*(1), 205–218.

Gautschi, W. and S. E. Notaris (1988). An algebraic study of Gauss–Kronrod quadrature formulae for Jacobi weight functions. *Math. Comp. 51*(183), 231–248.

Gautschi, W. and S. E. Notaris (1989). Gauss–Kronrod quadrature formulae for weight functions of Bernstein–Szegö type. *J. Comput. Appl. Math. 25*(2), 199–224. Erratum, *ibid. 27*(3) (1989), p. 429.

Gautschi, W. and T. J. Rivlin (1988). A family of Gauss–Kronrod quadrature formulae. *Math. Comp. 51*(184), 749–754.

Gautschi, W. and R. S. Varga (1983). Error bounds for Gaussian quadrature of analytic functions. *SIAM J. Numer. Anal. 20*(6), 1170–1186.

Gautschi, W. and J. Wimp (1987). Computing the Hilbert transform of a Jacobi weight function. *BIT 27*(2), 203–215.

Gautschi, W. and M. Zhang (1995). Computing orthogonal polynomials in Sobolev spaces. *Numer. Math. 71*(2), 159–183.

Gautschi, W., H. J. Landau, and G. V. Milovanović (1987). Polynomials orthogonal on the semicircle. II. *Constr. Approx. 3*(4), 389–404.

Gautschi, W., E. Tychopoulos, and R. S. Varga (1990). A note on the contour integral representation of the remainder term for a Gauss–Chebyshev quadrature rule. *SIAM J. Numer. Anal. 27*(1), 219–224.

Gautschi, W., L. Gori, and M. L. Lo Cascio (2000). Quadrature rules for rational functions. *Numer. Math. 86*(4), 617–633.

Golub, G. H. (1973a). Some modified matrix eigenvalue problems. *SIAM Rev. 15*(2), 318–334.

Golub, G. H. (1973b). Some uses of the Lanczos algorithm. In J. J. H. Miller (Ed.), *Topics in numerical analysis. Proc. Roy. Irish Acad. Conf., Univ. Coll., Dublin, 1972*, pp. 173–184. London: Academic Press.

Golub, G. H. and M. H. Gutknecht (1990). Modified moments for indefinite weight functions. *Numer. Math. 57*(6–7), 607–624.

Golub, G. H. and G. Meurant (1994). Matrices, moments and quadrature. In D. F. Griffiths and G. A. Watson (Eds), *Numerical analysis 1993 (Dundee, 1993)*, Volume 303 of *Pitman Res. Notes Math. Ser.*, pp. 105–156. Harlow: Longman Sci. Tech.

Golub, G. H. and Z. Strakoš (1994). Estimates in quadratic formulas. *Numer. Algorithms 8*(2–4), 241–268.

Golub, G. H. and U. von Matt (1991). Quadratically constrained least squares and quadratic problems. *Numer. Math. 59*(6), 561–580.

Golub, G. H. and J. H. Welsch (1969). Calculation of Gauss quadrature rules. *Math. Comp. 23*(106), 221–230. Loose microfiche suppl., A1–A10.

Gordon, R. G. (1968). Error bounds in equilibrium statistical mechanics. *J. Math. Phys. 9*(5), 655–663.

Gori, L. and C. A. Micchelli (1996). On weight functions which admit explicit Gauss–Turán quadrature formulas. *Math. Comp. 65*(216), 1567–1581.

Gori, L. and E. Santi (1992). Moment-preserving approximations: a monospline approach. *Rend. Mat. (7) 12*(4), 1031–1044.

Gori, L. and E. Santi (1995). On the evaluation of Hilbert transforms by means of a particular class of Turán quadrature rules. Special functions (Torino, 1993). *Numer. Algorithms 10*(1–2), 27–39.

Gori, L. and E. Santi (1999). Quadrature rules based on s-orthogonal polynomials for evaluating integrals with strong singularities. In W. Gautschi, G. H. Golub, and G. Opfer (Eds), *Applications and computation of orthogonal polynomials (Oberwolfach, 1998)*, Volume 131 of *Internat. Ser. Numer. Math.*, pp. 109–119. Basel: Birkhäuser.

Gori N. Amati, L. and E. Santi (1990). On a method of approximation by means of spline functions. In A. G. Law and C. L. Wang (Eds), *Approximation, optimization and computing*, pp. 41–46. Amsterdam: North-Holland.

Gradshteyn, I. S. and I. M. Ryzhik (2000). *Table of integrals, series, and products* (6th edn). San Diego, CA: Academic Press. Translated from the Russian. Translation edited and with a preface by Alan Jeffrey and Daniel Zwillinger.

Gragg, W. B. (1993). Positive definite Toeplitz matrices, the Arnoldi process for isometric operators, and Gaussian quadrature on the unit circle. Computational complex analysis. *J. Comput. Appl. Math. 46*(1–2), 183–198.

Gragg, W. B. and M. H. Gutknecht (1994). Stable look-ahead versions of the Euclidean and Chebyshev algorithms. In R. V. M. Zahar (Ed.), *Approximation and computation (West Lafayette, IN, 1993)*, Volume 119 of *Internat. Ser. Numer. Math.*, pp. 231–260. Boston, MA: Birkhäuser Boston.

Gragg, W. B. and W. J. Harrod (1984). The numerically stable reconstruction of Jacobi matrices from spectral data. *Numer. Math. 44*(3), 317–335.

Gröbner, W. (1967). Orthogonale Polynomsysteme, die gleichzeitig mit $f(x)$ auch deren Ableitung $f'(x)$ approximieren. In L. Collatz, G. Meinardus, and H. Unger (Eds), *Funktionalanalysis, Approximationstheorie, Numerische Mathematik (Oberwolfach, 1965)*, Volume 7 of *Internat. Ser. Numer. Math.*, pp. 24–32. Basel: Birkhäuser.

Groenevelt, W. G. M. (2002). Zeros of Sobolev orthogonal polynomials of Gegenbauer type. *J. Approx. Theory 114*(1), 115–140.

Hanke, M. (2003). A note on Tikhonov regularization of large problems. *BIT Numer. Math. 43*(2), 449–451.

Hansen, E. R. (1975). *A table of series and products*. Englewood Cliffs, NJ: Prentice-Hall.

Hardy, G. H. and J. E. Littlewood (1936). Notes on the theory of series (xx): on Lambert series. *Proc. London Math. Soc. (2) 41*, 257–270.

Henrici, P. (1986). *Applied and computational complex analysis. Volume 3. Discrete Fourier analysis—Cauchy integrals—construction of conformal maps—univalent functions*. Pure and Applied Mathematics. New York: John Wiley & Sons Inc.

Hestenes, M. R. and E. Stiefel (1952). Methods of conjugate gradients for solving linear systems. *J. Research Nat. Bur. Standards 49*(6), 409–436.

Hunter, D. B. (1970). Clenshaw's method for evaluating certain finite series. *Comput. J. 13*(4), 378–381.

Hunter, D. and G. Nikolov (2000). On the error term of symmetric Gauss–Lobatto quadrature formulae for analytic functions. *Math. Comp. 69*(229), 269–282.

Hunter, D. B. and G. E. Okecha (1986). A modified Gaussian quadrature rule for integrals involving poles of any order. *BIT 26*(2), 233–240.

Ixaru, L. G. and B. Paternoster (2001). A Gauss quadrature rule for oscillatory integrands. *Comput. Phys. Comm. 133*(2–3), 177–188.

Jacobi, C. G. J. (1826). Ueber Gaußs neue Methode, die Werthe der Integrale näherungsweise zu finden. *J. Reine Angew. Math. 1*, 301–308.

Jagels, C. and L. Reichel (1993). On the construction of Szegö polynomials. Computational complex analysis. *J. Comput. Appl. Math. 46*(1–2), 241–254.

Johnson, N. L., S. Kotz, and N. Balakrishnan (1995). *Continuous univariate distributions* (2nd edn), Volume 2 of *Wiley Series in Probability and Mathematical Statistics: Applied Probability and Statistics*. New York: Wiley.

Jones, W. B. and W. J. Thron (1980). *Continued fractions. Analytic theory and applications*, Volume 11 of *Encyclopedia of Mathematics and its Applications*. Reading, MA: Addison-Wesley Publ. Co. With a foreword by Felix E. Browder. With an introduction by Peter Henrici.

Jones, W. B., O. Njåstad, and W. J. Thron (1989). Moment theory, orthogonal polynomials, quadrature, and continued fractions associated with the unit circle. *Bull. London Math. Soc. 21*(2), 113–152.

Kahaner, D. K. and G. Monegato (1978). Nonexistence of extended Gauss–Laguerre and Gauss–Hermite quadrature rules with positive weights. *Z. Angew. Math. Phys. 29*(6), 983–986.

Kahaner, D., G. Tietjen, and R. Beckman (1982). Gaussian-quadrature formulas for $\int_0^\infty e^{-x^2} g(x)dx$. *J. Statist. Comput. Simulation 15*(2–3), 155–160.

Kahaner, D. K., J. Waldvogel, and L. W. Fullerton (1982). Addition of points to Gauss–Laguerre quadrature formulas. Tech. Report Series 8205, IMSL, Houston.

Kahaner, D. K., J. Waldvogel, and L. W. Fullerton (1984). Addition of points to Gauss–Laguerre quadrature formulas. *SIAM J. Sci. Statist. Comput. 5*(1), 42–55.

Kautsky, J. and S. Elhay (1984). Gauss quadratures and Jacobi matrices for weight functions not of one sign. *Math. Comp. 43*(168), 543–550.

Kautský, J. and G. H. Golub (1983). On the calculation of Jacobi matrices. *Linear Algebra Appl. 52/53*, 439–455.

King, H. F. and M. Dupuis (1976). Numerical integration using Rys polynomials. *J. Computational Phys. 21*(2), 144–165.

Kis, O. (1957). Remark on mechanical quadrature. *Acta Math. Acad. Sci. Hungar. 8*(3–4), 473–476.

Koornwinder, T. H. (1984). Orthogonal polynomials with weight function $(1-x)^\alpha(1+x)^\beta + M\delta(x+1) + N\delta(x-1)$. *Canadian Math. Bull. 27*(2), 205–213.

Korneĭčuk, A. A. (1964). Quadrature formulae for singular integrals. *Ž. Vyčisl. Mat. i Mat. Fiz. 4*(4), suppl., 64–74. Russian.

Kovačević, M. A. and G. V. Milovanović (1996). Spline approximation and generalized Turán quadratures. *Portugal. Math. 53*(3), 355–366.

Kripke, B. R. (1964). Best approximation with respect to nearby norms. *Numer. Math. 6*(2), 103–105.

Kronrod, A. S. (1965). *Nodes and weights of quadrature formulas. Sixteen-place tables*. New York: Consultants Bureau. Authorized translation from the Russian.

Laframboise, J. G. and A. D. Stauffer (1969). Optimum discrete approximation of the Maxwell distribution. *AIAAJ 7*(3), 520–523.

Lanczos, C. (1950). An iteration method for the solution of the eigenvalue problem of linear differential and integral operators. *J. Research Nat. Bur. Standards 45*(4), 255–282. Also in *Collected Published Papers with Commentaries*, Volume V, pp. 3-9–3-36.

Laščenov, K. V. (1953). On a class of orthogonal polynomials. *Leningrad. Gos. Ped. Inst. Uč. Zap. 89*, 167–189. Russian.

Laurie, D. P. (1992). Stratified sequences of nested quadrature formulas. *Quaestiones Math. 15*(3), 365–384.

Laurie, D. P. (1996). Anti-Gaussian quadrature formulas. *Math. Comp. 65*(214), 739–747.

Laurie, D. P. (1997). Calculation of Gauss–Kronrod quadrature rules. *Math. Comp. 66*(219), 1133–1145.

Laurie, D. P. (1999a). Accurate recovery of recursion coefficients from Gaussian quadrature formulas. Numerical evaluation of integrals. *J. Comput. Appl. Math. 112*(1–2), 165–180.

Laurie, D. P. (1999b). Questions related to Gaussian quadrature formulas and two-term recursions. In W. Gautschi, G. H. Golub, and G. Opfer (Eds), *Applications and computation of orthogonal polynomials (Oberwolfach, 1998)*, Volume 131 of *Internat. Ser. Numer. Math.*, pp. 133–144. Basel: Birkhäuser.

Laurie, D. P. (2001). Computation of Gauss-type quadrature formulas. Numerical analysis 2000, Vol. 5, Quadrature and orthogonal polynomials. *J. Comput. Appl. Math. 127*(1–2), 201–217.

Laurie, D. (2004). Calculation of Radau–Kronrod and Lobatto–Kronrod quadrature formulas. To be submitted.

Lether, F. G. (1977a). Modified quadrature formulas for functions with nearby poles. *J. Comput. Appl. Math. 3*(1), 3–9.

Lether, F. G. (1977b). Subtracting out complex singularities in numerical integration. *Math. Comp. 31*(137), 223–229.

Levin, E. and D. S. Lubinsky (2001). *Orthogonal polynomials for exponential weights*, Volume 4 of *CMS Books in Mathematics*. New York: Springer-Verlag.

Lewanowicz, S. (1979). Construction of a recurrence relation for modified moments. *J. Comput. Appl. Math. 5*(3), 193–206.

Lewanowicz, S. (1994a). A fast algorithm for the construction of recurrence relations for modified moments. *Appl. Math. (Warsaw) 22*(3), 359–372.

Lewanowicz, S. (1994b). A simple approach to the summation of certain slowly convergent series. *Math. Comp. 63*(208), 741–745.

Lewis, D. C. (1947). Polynomial least square approximations. *Amer. J. Math. 69*, 273–278.

Li, S. (1994). Kronrod extension of Turán formula. *Studia Sci. Math. Hungar. 29*(1–2), 71–83.

Li, S. (1996). Kronrod extension of generalized Gauss–Radau and Gauss–Lobatto formulae. *Rocky Mountain J. Math. 26*(4), 1455–1472.

Li, S. (1999). Construction and computation of a new set of orthogonal polynomials. In W. Gautschi, G. H. Golub, and G. Opfer (Eds), *Applications and computation of orthogonal polynomials (Oberwolfach, 1998)*, Volume 131 of *Internat. Ser. Numer. Math.*, pp. 145–151. Basel: Birkhäuser.

Lobatto, R. (1852). *Lessen over de Differentiaal- en Iintegraal-Rekening. Part II. Iintegraal-Rekening.* The Hague: Van Cleef.

López Lagomasino, G. and J. Illán (1984). A note on generalized quadrature formulas of Gauss–Jacobi type. In V. Sendov and V. Popov (Eds), *Constructive theory of functions*, pp. 513–518. Sofia: Publ. House Bulgarian Acad. Sci.

López Lagomasino, G. and J. Illán González (1987). Sobre los métodos interpolatorios de integración numérica y su conexión con la aproximación racional. *Cienc. Mat. (Havana) 8*(2), 31–44.

Luke, Y. L. (1969). *The special functions and their approximations. Volume II*, Volume 53 of *Mathematics in Science and Engineering.* New York: Academic Press.

Mach, R. (1984). Orthogonal polynomials with exponential weight in a finite interval and application to the optical model. *J. Math. Phys. 25*(7), 2186–2193.

Mantica, G. (1996). A stable Stieltjes technique for computing orthogonal polynomials and Jacobi matrices associated with a class of singular measures. *Constr. Approx. 12*(4), 509–530.

Mantica, G. (2000). On computing Jacobi matrices associated with recurrent and Möbius iterated function systems. Proceedings of the 8th International Congress on Computational and Applied Mathematics, ICCAM-98 (Leuven). *J. Comput. Appl. Math. 115*(1–2), 419–431.

Marcellán, F. and R. Álvarez–Nodarse (2001). On the "Favard theorem" and its extensions. Numerical analysis 2000, Vol. 5, Quadrature and orthogonal polynomials. *J. Comput. Appl. Math. 127*(1–2), 231–254.

Marcellán, F. and A. Ronveaux (1990). On a class of polynomials orthogonal with respect to a discrete Sobolev inner product. *Indag. Math. (N.S.) 1*(4), 451–464.

Marcellán, F. and A. Ronveaux (1995). Orthogonal polynomials and Sobolev inner products: a bibliography. Technical report, Laboratoire de Physique Mathématique, Facultés Universitaires N. D. de la Paix, Namur, Belgium.

Marcellán, F., M. Alfaro, and M. L. Rezola (1993). Orthogonal polynomials on Sobolev spaces: old and new directions. Proceedings of the Seventh Spanish Symposium on Orthogonal Polynomials and Applications (VII SPOA) (Granada, 1991). *J. Comput. Appl. Math. 48*(1–2), 113–131.

Marcellán, F., T. E. Pérez, M. A. Piñar, and A. Ronveaux (1996). General Sobolev orthogonal polynomials. *J. Math. Anal. Appl. 200*(3), 614–634.

Markoff, A. (1885). Sur la méthode de Gauss pour le calcul approché des intégrales. *Math. Ann. 25*, 427–432.

Mason, J. C. and D. C. Handscomb (2003). *Chebyshev polynomials*. Boca Raton, FL: Chapman & Hall/RCR.

McLellan IV, A. (1968). Tables of the Riemann zeta function and related functions. *Math. Comp. 22*(103), 687–688. Review 69.

Meijer, H. G. (1994). Sobolev orthogonal polynomials with a small number of real zeros. *J. Approx. Theory 77*(3), 305–313.

Meijer, H. G. (1996). A short history of orthogonal polynomials in a Sobolev space. I. The non-discrete case. *Nieuw Arch. Wisk. 14*(1), 93–112.

Micchelli, C. (1972). The fundamental theorem of algebra for monosplines with multiplicities. In P. L. Butzer, J.-P. Kahane, and B. Sz.–Nagy (Eds), *Linear operators and approximation*, Volume 20 of *Internat. Ser. Numer. Math.*, pp. 419–430. Basel: Birkhäuser.

Micchelli, C. A. (1988). Monosplines and moment preserving spline approximation. In H. Brass and G. Hämmerlin (Eds), *Numerical integration, III (Oberwolfach, 1987)*, Volume 85 of *Internat. Ser. Numer. Math.*, pp. 130–139. Basel: Birkhäuser.

Milovanović, G. V. (1988). Construction of s-orthogonal polynomials and Turán quadrature formulae. In G. V. Milovanović (Ed.), *Numerical methods and approximation III (Niš, 1987)*, pp. 311–328. Niš: Univ. Niš.

Milovanović, G. V. (2001). Quadratures with multiple nodes, power orthogonality, and moment-preserving spline approximation. Numerical analysis 2000, Vol. 5, Quadrature and orthogonal polynomials. *J. Comput. Appl. Math. 127*(1–2), 267–286.

Milovanović, G. V. (2002). Orthogonal polynomials on the radial rays in the complex plane and applications. Proceedings of the Fifth International Conference on Functional Analysis and Approximation Theory, Volume 1 (Potenza, 2000). *Rend. Circ. Mat. Palermo* (68), 65–94.

Milovanović, G. V. and A. Cvetković (2004). Orthogonal polynomials and Gaussian quadrature rules related to oscillatory weight functions. Submitted for publication.

Milovanović, G. V. and M. A. Kovačević (1988). Moment-preserving spline approximation and Turán quadratures. In R. P. Agarwal, Y. M. Chow, and S. J. Wilson (Eds), *Numerical mathematics, Singapore 1988*, Volume 86 of *Internat. Ser. Numer. Math.*, pp. 357–365. Basel: Birkhäuser.

Milovanović, G. V. and P. M. Rajković (1990). Geronimus concept of orthogonality for polynomials orthogonal on a circular arc. *Rend. Mat. Appl. (7) 10*(2), 383–390.

Milovanović, G. V. and P. M. Rajković (1994). On polynomials orthogonal on a circular arc. *J. Comput. Appl. Math. 51*(1), 1–13.

Milovanović, G. V. and M. M. Spalević (2002). Quadrature formulae connected to σ-orthogonal polynomials. Proceedings of the 9th International Congress on

Computational and Applied Mathematics (Leuven, 2000). *J. Comput. Appl. Math. 140*(1–2), 619–637.

Milovanović, G. V. and M. M. Spalević (2003). Error bounds for Gauss–Turán quadrature formulae of analytic functions. *Math. Comp. 72*(244), 1855–1872.

Milovanović, G. V. and M. Stanić (2003). Construction of multiple orthogonal polynomials by discretized Stieltjes–Gautschi procedure and corresponding Gaussian quadratures. *Facta Univ. (Niš), Ser. Math. Inform. 18*(1), 9–29.

Min, G. (1998a). Lagrange interpolation and quadrature formula in rational systems. *J. Approx. Theory 95*(1), 123–145.

Min, G. (1998b). Lobatto-type quadrature formula in rational spaces. *J. Comput. Appl. Math. 94*(1), 1–12.

Monegato, G. (1976). A note on extended Gaussian quadrature rules. *Math. Comp. 30*(136), 812–817.

Monegato, G. (1978a). Positivity of the weights of extended Gauss–Legendre quadrature rules. *Math. Comp. 32*(141), 243–245.

Monegato, G. (1978b). Some remarks on the construction of extended Gaussian quadrature rules. *Math. Comp. 32*(141), 247–252.

Monegato, G. (1979). An overview of results and questions related to Kronrod schemes. In G. Hämmerlin (Ed.), *Numerische Integration*, Volume 45 of *Internat. Ser. Numer. Math.*, pp. 231–240. Basel: Birkhäuser.

Monegato, G. (1982). Stieltjes polynomials and related quadrature rules. *SIAM Rev. 24*(2), 137–158.

Monegato, G. (2001). An overview of the computational aspects of Kronrod quadrature rules. *Numer. Algorithms 26*(2), 173–196.

Muskhelishvili, N. I. (1977). *Singular integral equations*. Leyden: Noordhoff International Publishing. Revised translation from the Russian, edited by J. R. M. Radok. Reprint of the 1958 edition.

Mysovskih, I. P. (1964). A special case of quadrature formulae containing preassigned nodes. *Vesci Akad. Navuk BSSR Ser. Fiz.-Tehn. Navuk 4*, 125–127. Russian.

Natanson, I. P. (1965). *Constructive function theory. Vol. II. Approximation in mean*. New York: Frederick Ungar Publishing Co. Translated from the Russian by John R. Schulenberger.

Nikiforov, A. F., S. K. Suslov, and V. B. Uvarov (1991). *Classical orthogonal polynomials of a discrete variable*. Springer Series in Computational Physics. Berlin: Springer-Verlag. Translated from the Russian.

Nikishin, E. M. and V. N. Sorokin (1991). *Rational approximations and orthogonality*, Volume 92 of *Translation of Mathematical Monographs*. Providence, RI: American Mathematical Society. Translated from the Russian by Ralph P. Boas.

Notaris, S. E. (1990). Gauss–Kronrod quadrature formulae for weight functions of Berstein–Szegö type. II. *J. Comput. Appl. Math. 29*(2), 161–169.

Notaris, S. E. (1994). An overview of results on the existence or nonexistence and the error term of Gauss–Kronrod quadrature formulae. In R. V. M. Zahar (Ed.), *Approximation and computation (West Lafayette, IN, 1993)*, Volume 119 of *Internat. Ser. Numer. Math.*, pp. 485–496. Boston, MA: Birkhäuser Boston.

Oliver, J. (1977). An error analysis of the modified Clenshaw method for evaluating Chebyshev and Fourier series. *J. Inst. Math. Appl. 20*(3), 379–391.

Ossicini, A. and F. Rosati (1978). Sulla convergenza dei funzionali ipergaussiani. *Rend. Mat. (6) 11*(1), 97–108.

Parlett, B. N. (1998). *The symmetric eigenvalue problem*, Volume 20 of *Classics in applied mathematics*. Philadelphia, PA: SIAM. Corrected reprint of the 1980 original.

Patterson, T. N. L. (1968). The optimum addition of points to quadrature formulae. *Math. Comp. 22*(104), 847–856. Loose microfiche suppl. D1–D5. Errata, *ibid. 23*(108) (1969), 892.

Patterson, T. N. L. (1973). Algorithm 468—algorithm for automatic numerical integration over a finite interval. *Comm. ACM 16*(11), 694–699.

Peherstorfer, F. (1990a). On Stieltjes polynomials and Gauss–Kronrod quadrature. *Math. Comp. 55*(192), 649–664.

Peherstorfer, F. (1990b). Weight functions admitting repeated positive Kronrod quadrature. *BIT 30*(1), 145–151.

Peherstorfer, F. and K. Petras (2000). Ultraspherical Gauss–Kronrod quadrature is not possible for $\lambda > 3$. *SIAM J. Numer. Anal. 37*(3), 927–948 (electronic).

Peherstorfer, F. and K. Petras (2003). Stieltjes polynomials and Gauss–Kronrod quadrature for Jacobi weight functions. *Numer. Math. 95*(4), 689–706.

Perron, O. (1957). *Die Lehre von den Kettenbrüchen. Band II: Analytisch-funktionentheoretische Kettenbrüche* (Third improved and enlarged edition). Stuttgart: B.G. Teubner Verlagsgesellschaft.

Petras, K. (1999). Positivity of Gauss–Kronrod formulae for a certain ultraspherical weight function. In W. Gautschi, G. H. Golub, and G. Opfer (Eds), *Applications and computation of orthogonal polynomials (Oberwolfach, 1998)*, Volume 131 of *Internat. Ser. Numer. Math.*, pp. 195–202. Basel: Birkhäuser.

Pichon, B. (1989). Numerical calculation of the generalized Fermi–Dirac integrals. *Comput. Phys. Comm. 55*(2), 127–136.

Pierrard, V. and A. Magnus (2003). Lorentzian orthogonal polynomials. Preprint.

Piessens, R. and M. Branders (1973). The evaluation and application of some modified moments. *Nordisk Tidskr. Informationsbehandling (BIT) 13*(4), 443–450.

Piessens, R. and M. Branders (1974). A note on the optimal addition of abscissas to quadrature formulas of Gauss and Lobatto type. *Math. Comp. 28*(125), 135–139. Supplement, *ibid.*, pp. 344–347.

Posse, C. (1875). Sur les quadratures. *Nouv. Ann. Math. 14*, 49–62.

Rabinowitz, P. (1980). The exact degree of precision of generalized Gauss–Kronrod integration rules. *Math. Comp. 35*(152), 1275–1283.

Radau, R. (1880). Étude sur les formules d'approximation qui servent à calculer la valeur numérique d'une intégrale définie. *J. Math. Pures Appl. 6*, 283–336.

Rees, C. J. (1945). Elliptic orthogonal polynomials. *Duke Math. J. 12*, 173–187.

Reichel, L. (1993). Construction of polynomials that are orthogonal with respect to a discrete bilinear form. *Adv. Comput. Math. 1*(2), 241–258.

Russon, A. E. and J. M. Blair (1969). Rational function minimax approximations for the Bessel functions $K_0(x)$ and $K_1(x)$. Rep. AECL-3461, Atomic Energy of Canada Limited, Chalk River, Ontario.

Rutishauser, H. (1957). Der Quotienten–Differenzen–Algorithmus. Number 7 of *Mitt. Inst. Angew. Math. Zürich*.

Rutishauser, H. (1963). On Jacobi rotation patterns. In N. C. Metropolis, A. H. Taub, J. Todd, and C. B. Tompkins (Eds), *Experimental arithmetics, high speed computing and mathematics*, Volume 15 of *Proc. Sympos. Appl. Math.*, pp. 219–239. Providence, RI: Amer. Math. Soc.

Sack, R. A. and A. F. Donovan (1969). An algorithm for Gaussian quadrature given generalized moments. Technical report, Dept. Math., Univ. of Salford, Salford, UK.

Sack, R. A. and A. Donovan (1972). An algorithm for Gaussian quadrature given modified moments. *Numer. Math. 18*(5), 465–478.

Saffren, M. M. and E. W. Ng (1971). Recursive algorithms for the summation of certain series. *SIAM J. Math. Anal. 2*(1), 31–36.

Sagar, R. P. (1991). A Gaussian quadrature for the calculation of generalized Fermi–Dirac integrals. *Comput. Phys. Comm. 66*(2–3), 271–275.

Salzer, H. E. (1973). A recurrence scheme for converting from one orthogonal expansion into another. *Comm. ACM 16*(1), 705–707.

Saylor, P. E. and D. C. Smolarski (2001). Why Gaussian quadrature in the complex plane? *Numer. Algorithms 26*(3), 251–280. See also Addendum, *ibid. 27*(2) (2001), pp. 215–217.

Scherer, R. and T. Schira (2000). Estimating quadrature errors for analytic functions using kernel representations and biorthogonal systems. *Numer. Math. 84*(3), 497–518.

Schira, T. (1994). *Ableitungsfreie Fehlerabschätzungen bei numerischer Integration holomorpher Funktionen*. Ph.D. thesis, Universität Karlsruhe, Karlsruhe.

Schira, T. (1996). The remainder term for analytic functions of Gauss–Lobatto quadratures. *J. Comput. Appl. Math. 76*(1–2), 171–193.

Schira, T. (1997). The remainder term for analytic functions of symmetric Gaussian quadratures. *Math. Comp. 66*(217), 297–310.

Schoutens, W. (2000). *Stochastic processes and orthogonal polynomials*, Volume 146 of *Lecture Notes in Statistics*. New York: Springer-Verlag.

Shi, Y. G. (1996). Generalized Gaussian Kronrod–Turán quadrature formulas. *Acta Sci. Math. (Szeged) 62*(1–2), 175–185.

Shizgal, B. (1979). Eigenvalues of the Lorentz Fokker–Planck equation. *J. Chem. Phys. 70*(4), 1948–1951.

Shizgal, B. (1981). A Gaussian quadrature procedure for use in the solution of the Boltzmann equation and related problems. *J. Comput. Phys. 41*(2), 309–328.

Shohat, J. A. and J. D. Tamarkin (1943). *The problem of moments*, Volume 2 of *AMS Mathematical Surveys*. New York: American Mathematical Society.

Sinap, A. and W. Van Assche (1996). Orthogonal matrix polynomials and applications. Proceedings of the Sixth International Congress on Computational and Applied Mathematics (Leuven, 1994). *J. Comput. Appl. Math. 66*(1–2), 27–52.

Smith, F. J. (1965). An algorithm for summing orthogonal polynomial series and their derivatives with applications to curve-fitting and interpolation. *Math. Comp. 19*(89), 33–36.

Smoktunowicz, A. (2002). Backward stability of Clenshaw's algorithm. *BIT 42*(3), 600–610.

Spalević, M. M. (2002). Quadrature formulae of Radau and Lobatto type connected to s–orthogonal polynomials. *Zh. Vychisl. Mat. Mat. Fiz. 42*(5), 615–626. Reprinted in Comput. Math. Math. Phys. 42 (2002), 587–598.

Stahl, H. and V. Totik (1992). *General orthogonal polynomials*, Volume 43 of *Encyclopedia of Mathematics and Its Applications*. Cambridge: Cambridge Univ. Press.

Steen, N. M., G. D. Byrne, and E. M. Gelbard (1969). Gaussian quadratures for the integrals $\int_0^\infty \exp(-x^2) f(x)dx$ and $\int_0^b \exp(-x^2) f(x)dx$. *Math. Comp. 23*(107), 661–671. See also Editorial Remarks and Note by Milton R. Pine, *ibid.*, pp. 673–674.

Stiefel, E. L. (1958). Kernel polynomials in linear algebra and their numerical applications. In *Further contributions to the solution of simultaneous linear equations and the determination of eigenvalues*, Volume 49 of *Nat. Bur. Standards Appl. Math. Ser.*, pp. 1–22. Washington, DC: U.S. Government Printing Office.

Stieltjes, T. J. (1884). Quelques recherches sur la théorie des quadratures dites mécaniques. *Ann. Sci. École Norm. Paris, Sér. 3 1*, 409–426. Also in *Œuvres I*, pp. 377–396.

Stroud, A. H. and D. D. Stancu (1965). Quadrature formulas with multiple Gaussian nodes. *J. Soc. Indust. Appl. Math. Ser. B Numer. Anal. 2*(1), 129–143.

Suetin, P. (1979). *Classical orthogonal polynomials* (2nd edn). Moscow: "Nauka". Russian.

Swarztrauber, P. N. (2002). On computing the points and weights for Gauss–Legendre quadrature. *SIAM J. Sci. Comput. 24*(3), 945–954.

Szegö, G. (1935). Über gewisse orthogonale Polynome, die zu einer oszillierenden Belegungsfunktion gehören. *Math. Ann. 110*, 501–513. Also in Collected Papers (R. Askey, ed.), Vol. 2, 545–557.

Szegö, G. (1975). *Orthogonal polynomials* (Fourth ed.), Volume 23 of *AMS Colloquium Publications*. Providence, RI: Amer. Math. Soc.

Todd, J. (1954). The condition of the finite segments of the Hilbert matrix. In *Contributions to the solution of systems of linear equations and the determination of eigenvalues*, Volume 39 of *Nat. Bur. Standards Appl. Math. Ser.*, pp. 109–116. Washington, DC: U.S. Government Printing Office.

Turán, P. (1950). On the theory of the mechanical quadrature. *Acta Sci. Math. Szeged 12* (Part A), 30–37.

Uvarov, V. B. (1959). Relation between polynomials orthogonal with different weights. *Dokl. Akad. Nauk SSSR 126*(1), 33–36. Russian.

Uvarov, V. B. (1969). The connection between systems of polynomials that are orthogonal with respect to different distribution functions. *Ž. Vyčisl. Mat. i Mat. Fiz. 9*(6), 1253–1262. Russian. English translation in *U.S.S.R. Comput. Math. Math. Phys. 9*(6) (1969), pp. 25–36.

Van Assche, W. (1987). *Asymptotics for orthogonal polynomials*, Volume 1265 of *Lecture Notes in Math.* Berlin: Springer-Verlag.

Van Assche, W. (1991). Orthogonal polynomials, associated polynomials and functions of the second kind. *J. Comput. Math. Appl. 37*(1–3), 237–249.

Van Assche, W. and E. Coussement (2001). Some classical multiple orthogonal polynomials. Numerical analysis 2000, Vol. 5, Quadrature and orthogonal polynomials. *J. Comput. Appl. Math. 127*(1–2), 317–347.

Van Assche, W. and I. Vanherwegen (1993). Quadrature formulas based on rational interpolation. *Math. Comp. 61*(204), 765–783.

Velamparambil, S. (1998). Email message to the author, December 17.

Verlinden, P. (1999). Stable rational modification of a weight. *Numer. Algorithms 22*(2), 183–192.

Weideman, J. A. C. and D. P. Laurie (2000). Quadrature rules based on partial fraction expansions. Computational methods from rational approximation theory (Wilrijk, 1999). *Numer. Algorithms 24*(1–2), 159–178.

Wheeler, J. C. (1974). Modified moments and Gaussian quadratures. Proceedings of the International Conference of Padé Approximants, Continued Fractions and Related Topics (Univ. Colorado, Boulder, CO, 1972, dedicated to the memory of H. S. Wall). *Rocky Mountain J. Math. 4*(2), 287–296.

Wheeler, J. C. (1984). Modified moments and continued fraction coefficients for the diatomic linear chain. *J. Chem. Phys. 80*(1), 472–476.

Wheeler, J. C. and C. Blumstein (1972). Modified moments for harmonic solids. *Phys. Rev. B6*, 4380–4382.

Wilf, H. S. (1978). *Mathematics for the physical sciences*. Dover Books in Advanced Mathematics. New York: Dover Publications, Inc. Reprint of the 1962 original.

Wilf, H. (1980). Personal communication.

Wimp, J. (1981). *Sequence transformations and their applications*, Volume 154 of *Mathematics in Science and Engineering*. New York: Academic Press, Inc.

Wimp, J. (1984). *Computation with recurrence relations*. Applicable Mathematics Series. Boston, MA: Pitman Advanced Publishing Program.

Wong, R. (1982). Quadrature formulas for oscillatory integral transforms. *Numer. Math. 39*(3), 351–360.

Wong, R. (1989). *Asymptotic approximations of integrals*. Computer Science and Scientific Computing. Boston, MA: Academic Press.

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