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Chapter 3

- Chapter 1 $\to$ 1-step methods: given $\vec{y}_n$ we can find $\vec{y}_{n+1}$
  - Explicit $\to$ order 1
  - Implicit $\to$ order 2
- Chapter 2 $\to$ multi-step methods: s-step
  - Explicit $\to$ order s
  - Implicit $\to$ order s+1
  - we need $y_n, y_{n+1}, y_{n+2}, \dots, y_{n+s-1}$ to find y_{n+s}
- Chapter 3
  - given $\vec{y}_n$ find $\vec{y}_{n+1}$, higher order method } Runge-Kutta Methods

§3.1 Gaussian Quadrature

Def a weight function ω is a nonnegative function on the interval $[a,b]$ such that:

i) $0 < \int_a^b \omega(\tau)\,d\tau < \infty$

ii) $\left|\int_a^b \tau^j \omega(\tau)\,d\tau\right| < \infty, \quad j = 1, 2, 3, \dots$

Goal: Find $b_1, b_2, b_3, \dots, b_\nu$ and $c_1, c_2, \dots, c_\nu$ such that

$$\int_a^b f(\tau)\omega(\tau)\,d\tau \approx \sum_{j=1}^{\nu} b_j f(c_j) \quad \text{(quadrature formula)}$$

is a good approximation.

- b_i's and c_i's are independent of f but they depend on ω and a,b
- b_i's are called quadrature weights
- c_i's are called quadrature nodes

How good is the approximation?

- Let $\hat{f}$ be a polynomial of degree $p-1$
- Suppose b_j's and c_j's are such that

$$\int_a^b \hat{f}(\tau)\omega(\tau)d\tau = \sum_{j=1}^{\upsilon} b_j \hat{f}(c_j)$$

- It can be shown that if f is a function with p smooth derivatives then

$$\left| \int_a^b f(\tau)\omega(\tau)d\tau - \sum_{j=1}^{\upsilon} b_j f(c_j) \right| \leq \alpha \max_{a\leq x\leq b} \left| f^{(p)}(x) \right| \qquad (\alpha \text{ constant} > 0)$$

$\Rightarrow$ the quadrature formula is of order p

The quadrature rule is of order p if it is <u>exact</u> for every $f \in \mathbb{P}_{p-1}$

$\mathbb{P}_m$ is the space of polynomials of degree m.

How to choose b_j's and c_j's?

Lemma 3.1: Given any distinct set of nodes $c_1, c_2, \ldots, c_\upsilon$, it is possible to find a unique set of weights $b_1, b_2, \ldots, b_\upsilon$ such that the quadrature formula is of order $p \geq \upsilon$.

Proof: We know that the quadrature formula is of order υ if it is exact for functions in $\mathbb{P}_{\upsilon-1}$. Take the basis for $\mathbb{P}_{\upsilon-1}$: $\{1, t, t^2, \ldots, t^{\upsilon-1}\}$. Then the following is true:

$$\sum_{j=1}^{\upsilon} b_j f_m(c_j) = \sum_{j=1}^{\upsilon} b_j c_j^m = \int_a^b \tau^m \omega(\tau)d\tau, \quad m = 0,1,2,\ldots,\upsilon-1 \qquad (f_m(\tau) = \tau^m)$$

This is a system of υ equations for υ unknowns, $(b_1, b_2, \ldots, b_\upsilon)$

$$\underbrace{\begin{bmatrix} 1 & 1 & 1 & 1 & \cdots & 1 \\ c_1 & c_2 & c_3 & c_4 & \cdots & c_\upsilon \\ c_1^2 & c_2^2 & c_3^2 & c_4^2 & \cdots & c_\upsilon^2 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ c_1^{\upsilon-1} & c_2^{\upsilon-1} & c_3^{\upsilon-1} & c_4^{\upsilon-1} & \cdots & c_\upsilon^{\upsilon-1} \end{bmatrix}}_{\text{Vandermonde Matrix}} \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ \vdots \\ b_\upsilon \end{bmatrix} = \begin{bmatrix} \int_a^b \omega(\tau)d\tau \\ \int_a^b \omega(\tau)\tau d\tau \\ \int_a^b \omega(\tau)\tau^2 d\tau \\ \vdots \\ \int_a^b \omega(\tau)\tau^{\upsilon-1}d\tau \end{bmatrix}$$

It's determinant is non-zero if and only if $c_i \neq c_j$ for $i \neq j$. The inverse in our case exists. ∎

Alternative to finding b_j's: Use Lagrange interpolation polynomials. Define

$$p_j(t) = \prod_{\substack{k=1 \\ k\neq j}}^{\upsilon} \frac{t - c_k}{c_j - c_k}, \quad j = 1,2,\ldots,\upsilon$$

Reminder: $p_j(c_j)=1$, $p_j(c_m)=0$ if $m\neq j$.
If g is a polynomial of degree $\upsilon-1$ then

$$\sum_{j=1}^{\upsilon} p_j(t)\,g(c_j) = g(t).$$

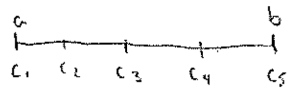
It follows that

$$\int_a^b \tau^m \omega(\tau)\,d\tau \underset{\uparrow}{=} \int_a^b \left(\sum_{j=1}^{\upsilon} p_j(\tau)\,c_j^m\right)\omega(\tau)\,d\tau = \sum_{j=1}^{\upsilon}\left(\int_a^b p_j(\tau)\omega(\tau)\,d\tau\right)c_j^m = \sum_{j=1}^{\upsilon} b_j c_j^m$$

$$\left(\tau^m = g(\tau) = \sum_{j=1}^{\upsilon} p_j(\tau)\,g(c_j)\right)$$

$$\Longrightarrow b_j = \int_a^b p_j(\tau)\omega(\tau)\,d\tau, \quad j=1,2,\ldots,\upsilon.$$

$$\int_a^b f(\tau)\omega(\tau)\,d\tau \approx \sum_{j=1}^{\upsilon} b_j f(c_j)$$



possible but not recommended

Goal: Choose c_j's such that we have as high order as possible.

Definitions:

1) On the interval (a,b) define the inner product

$$\langle f,g\rangle := \int_a^b f(\tau)g(\tau)\omega(\tau)\,d\tau$$

where $\omega(\tau)$ is a weight function and f and g such that

$$\int_a^b (f(\tau))^2\,d\tau < \infty, \quad \int_a^b (g(\tau))^2\,d\tau < \infty.$$

2) A polynomial $p_m \in \mathbb{P}_m$, $p_m \neq 0$, is an m^{th} orthogonal polynomial (with respect to ω) if $\langle p_m, \hat{p}\rangle = 0 \quad \forall \hat{p} \in \mathbb{P}_{m-1}$

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A property of orthogonal polynomials p_m is that all m zeros lie in the interval (a,b) and they are simple

Proof: p_m is an orthogonal polynomial so $\langle p_m, \hat{p}\rangle = 0 \quad \forall \hat{p}\in\mathbb{P}_{m-1}$, so

$$\langle p_m, 1\rangle = 0 \iff \int_a^b p_m(\tau)\omega(\tau)\,d\tau = 0.$$

It follows that p_m has to change sign at least once on (a,b). Denote by $x_1,\dots,x_k$ all the points in (a,b) where p_m changes sign (we already know that $k \geq 1$). Assume that $k \leq m-1$. Define

$$q(t) = \prod_{j=1}^{k}(t-x_j) = \sum_{i=0}^{k} q_i t^i.$$

Then p_m and q change sign in (a,b) in exactly the same points. Thus the sign of $p_m q$ does not change on (a,b). Since $\omega(t) \geq 0$ and $p_m q \neq 0$ we have

$$\int_a^b p_m(\tau) q(\tau) \omega(\tau) d\tau \neq 0.$$

But $p_m(t)$ is an orthogonal polynomial so

$$\int_a^b p_m(\tau) q(\tau) \omega(\tau) d\tau = \sum_{i=0}^{k} q_i \langle p_m, t^i \rangle = 0$$

as $t^i \in \mathbb{P}_{m-1}$. This is a contradiction so $k \geq m$. But every polynomial $\hat{p} \in \mathbb{P}_m \setminus \mathbb{P}_{m-1}$ have exactly m zeros. Thus $k=m$. ∎

Theorem 3.3: Let $c_1, c_2, \dots, c_\nu$ be zeros of the orthogonal polynomial p_ν. Let $b_1, b_2, \dots, b_\nu$ be the weights that can be computed by lemma 3.1 (Vandermonde system). Then:

1) The quadrature method is of order 2ν
2) There is no other quadrature method of higher order.

Proof: Let $\hat{p} \in \mathbb{P}_{2\nu-1}$. It is possible to find polynomials $q, r \in \mathbb{P}_{\nu-1}$ such that $\hat{p} = p_\nu q + r$. It follows that

$$\begin{aligned}\int_a^b \hat{p}(\tau)\omega(\tau)d\tau &= \int_a^b p_\nu(\tau) q(\tau) \omega(\tau) d\tau + \int_a^b r(\tau)\omega(\tau)d\tau \\ &= \cancel{\langle p_\nu, q \rangle}^{\,0} + \int_a^b r(\tau)\omega(\tau)d\tau \\ &= \int_a^b r(\tau)\omega(\tau)d\tau\end{aligned}$$

We also have

$$\sum_{j=1}^{\nu} b_j \hat{p}(c_j) = \sum_{j=1}^{\nu} b_j \underbrace{p_\nu(c_j)}_{=0} q(c_j) + \sum_{j=1}^{\nu} b_j r(c_j) = \sum_{j=1}^{\nu} b_j r(c_j).$$

We know that $r \in \mathbb{P}_{\nu-1}$ and therefore

$$\sum_{j=1}^{\nu} b_j r(c_j) = \int_a^b r(\tau)\omega(\tau)d\tau.$$

Now

$$\int_a^b \hat{p}(\tau)\omega(\tau)d\tau = \int_a^b r(\tau)\omega(\tau)d\tau = \sum_{j=1}^{\nu} b_j r(c_j) = \sum_{j=1}^{\nu} b_j \hat{p}(c_j).$$

So the quadrature formula is exact for $\hat{p} \in \mathbb{P}_{2\nu-1}$. Thus it is of order at least $p = 2\nu$. We still need to prove that order is exactly 2ν. We do this by contradiction. Assume that b_i's and c_i's are such that quadrature formula is of order $p \geq 2\nu+1$. Let

$$\hat{p}(t) = \prod_{i=1}^{\nu} (t-c_i)^2 \in \mathbb{P}_{2\nu}.$$

Then

$$\int_a^b \hat{p}(\tau)\omega(\tau)d\tau = \int_a^b \left(\prod_{i=1}^{\nu} (t-c_i)^2\right)\omega(t) > 0$$

and

$$\sum_{j=1}^{\nu} b_j \hat{p}(c_j) = \sum_{j=1}^{\nu} b_j \prod_{i=1}^{\nu} (c_j - c_i)^2 = 0.$$

So

$$\int_a^b \hat{p}(\tau)\omega(\tau)d\tau \neq \sum_{j=1}^{\nu} b_j \hat{p}(c_j)$$

and therefore the quadrature rule is <u>not</u> exact for polynomials in $\mathbb{P}_{2\nu}$ and therefore <u>cannot</u> be of order $p \geq 2\nu+1$. ∎

Theorem 3.4: Let $r \in \mathbb{P}_\nu$ obey the orthogonality conditions

- $\langle r, \hat{p} \rangle = 0 \quad \forall \hat{p} \in \mathbb{P}_{m-1}$
- $\langle r, t^m \rangle \neq 0$ for $m \in \{0,1,2,\ldots,\nu\}$
- Choose c_i's to be the zeros of polynomial r
- Compute b_j's from the Vandermonde system

Then the quadrature formula is of order $p = \nu + m$.

Runge-Kutta Methods

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Is it possible to find a higher order method to approximate $\vec{y}_{n+1}$ given $\vec{y}_n$? $\rightarrow$ RK methods

$$\vec{y}'(t) = \vec{f}(t, \vec{y}(t))$$

Integrate in time from t_n to t_{n+1}

$$\int_{t_n}^{t_{n+1}} \vec{y}'(t)dt = \int_{t_n}^{t_{n+1}} \vec{f}(t, \vec{y}(t))dt$$

$$\Rightarrow \vec{y}(t_{n+1}) = \vec{y}(t_n) + \int_{t_n}^{t_{n+1}} \vec{f}(t, \vec{y}(t))dt = \vec{y}(t_n) + h\int_0^1 \vec{f}(t_n + h\tau, \vec{y}(t_n + h\tau))d\tau$$

Use quadrature formula to approximate integral

$$\int_0^1 \vec{f}(t_n + h\tau, \vec{y}(t_n + h\tau))d\tau \approx \sum_{j=1}^{\nu} b_j \vec{f}(t_n + c_j h, \vec{y}(t_n + c_j h))$$

$$\vec{y}_{n+1} = \vec{y}_n + h\sum_{j=1}^{\nu} b_j \vec{f}(t_n + c_j h, \vec{y}(t_n + c_j h)), \quad n = 0, 1, 2, \dots$$

We need to approximate $\vec{y}(t_n + c_j h)$, $j = 1, 2, \dots, \nu$. We denote this approximation by $k_j \approx \vec{y}(t_n + c_j h)$, $j = 1, 2, \dots, \nu$. Choose $c_1 = 0$. Then $\vec{k}_1 = \vec{y}_n \approx \vec{y}(t_n + 0h)$. All the other $\vec{k}_j$'s will be chosen such that they are linear combinations of $\vec{f}(t_n + c_k h, \vec{k}_k)$, $k = 1, 2, \dots, \nu - 1$.

$$\vec{k}_1 = \vec{y}_n$$
$$\vec{k}_2 = \vec{y}_n + h a_{2,1} \vec{f}(t_n, \vec{k}_1)$$
$$\vec{k}_3 = \vec{y}_n + h a_{3,1} \vec{f}(t_n, \vec{k}_1) + h a_{3,2} \vec{f}(t_n, \vec{k}_2)$$

$$\vec{k}_\nu = \vec{y}_n + h\sum_{i=1}^{\nu-1} a_{\nu,i} \vec{f}(t_n + c_i h, \vec{k}_i)$$

With the $\vec{k}$'s given we can find $\vec{y}_{n+1}$:

$$\vec{y}_{n+1} = \vec{y}_n + h\sum_{j=1}^{\nu} b_j \vec{f}(t_n + c_j h, \vec{k}_j).$$

This is a RK method with ν-stages. Explicit Runge Kutta $\Rightarrow$ ERK.

The Runge-Kutta methods are defined by 3 sets of parameters

- the RK matrix $A \in \mathbb{R}^{\nu \times \nu}$ with elements $a_{j,i}$ $(j, i = 1, \dots, \nu)$
- the RK weights $\vec{b} \in \mathbb{R}^{\nu}$ with elements b_i
- the RK nodes $\vec{c} \in \mathbb{R}^{\nu}$ with elements c_i

A popular way of describing RK methods is by using the RK tableau (Butcher Tableau)

$$\begin{array}{c|c} \vec{c} & A \\ \hline & \vec{b}^T \end{array} \qquad \text{example:} \quad \begin{array}{c|cc} 0 & & \\ \frac{2}{3} & \frac{2}{3} & \\ \hline & \frac{1}{4} & \frac{1}{4} \end{array}$$

<u>Example</u> 2-stage RK-method $(\nu = 2)$

$$\vec{k}_1 = \vec{y}_n$$
$$\vec{k}_2 = \vec{y}_n + h a_{2,1} \vec{f}(t_n, \vec{k}_1)$$
$$\vec{y}_{n+1} = \vec{y}_n + h b_1 \vec{f}(t_n, \vec{k}_1) + h b_2 \vec{f}(t_n + c_2 h, \vec{k}_2)$$

Taylor expand:

$$\vec{f}(t_n + c_2 h, \vec{k}_2) = \vec{f}(t_n + c_2 h, \vec{y}_n + a_{2,1} h \vec{f}(t_n, \vec{y}_n))$$
$$= \vec{f}(t_n, \vec{y}_n) + h\left(c_2 \frac{\partial \vec{f}}{\partial t}(t_n, \vec{y}_n) + a_{2,1} \frac{\partial \vec{f}}{\partial \vec{y}}(t_n, \vec{y}_n) \vec{f}(t_n, \vec{y}_n)\right) + O(h^2)$$

$$\vec{y}_{n+1} = \vec{y}_n + h b_1 \vec{f}(t_n, \vec{k}_1) + h b_2 \vec{f}(t_n, \vec{y}_n) + h^2 b_2 \left(c_2 \frac{\partial \vec{f}}{\partial t}(t_n, \vec{y}_n) + a_{2,1} \frac{\partial \vec{f}}{\partial \vec{y}}(t_n, \vec{y}_n) \vec{f}(t_n, \vec{y}_n)\right) + O(h^3)$$

Now look at our ODE: $\vec{y}'(t) = \vec{f}(t, \vec{y}(t))$. Differentiating:

$$\vec{y}''(t) = \frac{\partial \vec{f}}{\partial t}(t, \vec{y}) + \frac{\partial \vec{f}}{\partial \vec{y}} \frac{\partial \vec{y}}{\partial t} = \frac{\partial \vec{f}}{\partial t}(t, \vec{y}) + \frac{\partial \vec{f}}{\partial \vec{y}} f(t, \vec{y}).$$

Let $\tilde{y}$ be the exact solution to

$$\tilde{y}'(t) = f(t, \tilde{y}(t)), \quad \underline{t \geq t_n}, \quad \tilde{y}(t_n) = \vec{y}_n$$

Then $\tilde{y}(t_{n+1})$ is the exact solution at $t = t_{n+1}$. Taylor expand:

$$\tilde{y}(t_{n+1}) = \tilde{y}(t_n) + h\tilde{y}' + \tfrac{1}{2} h^2 \tilde{y}'' + O(h^3)$$
$$= \vec{y}_n + h y' + \tfrac{1}{2} h^2 y'' + O(h^3)$$
$$= \vec{y}_n + h \vec{f}(t_n, \vec{y}_n) + \tfrac{1}{2} h^2 \left(\frac{\partial \vec{f}}{\partial t} + \frac{\partial \vec{f}}{\partial \vec{y}} \vec{f}(t_n, \vec{y}_n)\right) + O(h^3).$$

For terms to match for order $p = 2$ we need:

$$b_1 + b_2 = 1, \qquad c_2 b_2 = \tfrac{1}{2}, \qquad a_{2,1} = c_2$$

Popular choices:

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$$\begin{array}{c|cc} 0 & & \\ \frac{1}{2} & \frac{1}{2} & \\ \hline & 0 & 1 \end{array} \qquad \begin{array}{c|cc} 0 & & \\ \frac{2}{3} & \frac{2}{3} & \\ \hline & \frac{1}{4} & \frac{3}{4} \end{array} \qquad \begin{array}{c|cc} c_1 & & \\ c_2 & a_{2,1} & \\ \hline & b_1 & b_2 \end{array}$$

- RK method corresponding to

$$\begin{array}{c|cc} 0 & & \\ \frac{2}{3} & \frac{2}{3} & \\ \hline & \frac{1}{4} & \frac{3}{4} \end{array} \Rightarrow \quad \begin{array}{lll} c_1 = 0 & b_1 = \frac{1}{4} & \\ c_2 = \frac{2}{3} & b_2 = \frac{3}{4} & a_{2,1} = \frac{2}{3} \end{array}$$

$$\Rightarrow \vec{k}_1 = \vec{y}_n$$
$$\vec{k}_2 = \vec{y}_n + \tfrac{2}{3} h \vec{f}(t_n, \vec{k}_1)$$
$$\vec{y}_{n+1} = \vec{y}_n + \tfrac{1}{4} h \vec{f}(t_n, \vec{k}_1) + \tfrac{3}{4} h \vec{f}(t_n + \tfrac{3}{4}h, \vec{k}_2)$$

For a RK method to be of order at least 1 we need
$$\sum_{i=1}^{\nu-1} a_{j,i} = c_j, \quad j = 1, 2, \ldots, \nu$$
For order $p \le 3$ it is sufficient to consider $\underline{\text{autonomous scalar ODEs}}$
$\uparrow$ no t $\uparrow y \in \mathbb{R}^1$

$$y' = f(y), \; t \ge t_0, \; y(t_0) = y_0.$$
Notation: all functions evaluated at $t = t_n$ we drop subscript n
$$t_n \to t, \quad y_n \to y, \quad f(y_n) \to f$$

$$k_1 = y \longrightarrow f(k_1) = f(y) = f$$
$$k_2 = y + hc_2 f \longrightarrow f(k_2) = f(y + hc_2 f) \qquad (a_{2,1} = c_2)$$
$$= f + hc_2 f_y f + \tfrac{1}{2} h^2 c_2^2 f_{yy} f^2 + \mathcal{O}(h^3)$$
$$k_3 = y + ha_{3,1} f(k_1) + ha_{3,2} f(k_2)$$
$$= y + h(c_3 - a_{3,2}) f(k_1) + ha_{3,2} f(k_2) \qquad (a_{3,1} + a_{3,2} = c_3)$$
$$= y + h(c_3 - a_{3,2}) f + ha_{3,2}(f + hc_2 f_y f + \mathcal{O}(h^2))$$
$$= y + hc_3 f + h^2 a_{3,2} c_2 f_y f + \mathcal{O}(h^3)$$
$$\longrightarrow f(k_3) = f(y + hc_3 f + h^2 a_{3,2} c_2 f_y f + \mathcal{O}(h^3))$$
$$= f + (hc_3 f + h^2 a_{3,2} c_2 f_y f) f_y + \tfrac{1}{2}(hc_3 f + h^2 a_{3,2} c_2 f_y f)^2 f_{yy} + \mathcal{O}(h^3)$$
$$= f + hc_3 f_y f + h^2 \left(\tfrac{1}{2} c_3^2 f_{yy} f^2 + a_{3,2} c_2 f_y^2 f\right) + \mathcal{O}(h^3)$$

$$y_{n+1} = y + hb_1 f + hb_2 f(k_2) + hb_3 f(k_3)$$
$$= y + h(b_1 + b_2 + b_3) f + h^2 (c_2 b_2 + c_3 b_3) f_y f + h^3 \left(\tfrac{1}{2}(b_2 c_2^2 + b_3 c_3^2) f_{yy} f^2 + b_3 a_{3,2} c_2 f_y^2 f\right) + \mathcal{O}(h^4)$$

We can do a Taylor series expansion of $\tilde{y}$
$$\tilde{y}(t_{n+1}) = \tilde{y}(t_n) + h\tilde{y}'(t_n) + \tfrac{1}{2} h^2 \tilde{y}''(t_n) + \tfrac{1}{6} h^3 \tilde{y}'''(t_n) + \mathcal{O}(h^4)$$
But:
$$\tilde{y}' = f$$
$$\tilde{y}'' = f' = f_y f$$
$$\tilde{y}''' = f'' = (f_y f)' = f_{yy} f^2 + (f_y)^2 f$$

So

$$\tilde{y}(t_{n+1}) = y + hf + \tfrac{1}{2}h^2 f_y f + \tfrac{1}{6}h^3\left(f_{yy}f^2 + f_y^2 f\right) + O(h^4)$$

Match RK terms with the above:

- $b_1 + b_2 + b_3 = 1$
- $c_2 b_2 + c_3 b_3 = \frac{1}{2}$
- $b_2 c_2^2 + b_3 c_3^2 = \frac{1}{3}$
- $b_3 a_{3,2} c_2 = \frac{1}{6}$

Some important 3-stage methods

$$\begin{array}{c|ccc} 0 & & & \\ \frac{1}{2} & \frac{1}{2} & & \\ 1 & -1 & 2 & \\ \hline & \frac{1}{6} & \frac{2}{3} & \frac{1}{6} \end{array} \qquad\qquad \begin{array}{c|ccc} 0 & & & \\ \frac{2}{3} & \frac{2}{3} & & \\ \frac{2}{3} & 0 & \frac{2}{3} & \\ \hline & \frac{1}{4} & \frac{3}{8} & \frac{3}{8}\,? \end{array}$$

classical RK — Nystrom method

This is everything we will do on explicit RK methods

§3.3. Implicit RK (IRK)

$$\left.\begin{aligned} \vec{k}_1 &= \vec{y}_n \\ \vec{k}_2 &= \vec{y}_n + h a_{2,1} \vec{f}(t_n, \vec{k}_1) \\ &\vdots \\ \vec{k}_v &= \vec{y}_n + h\sum_{j=1}^{v} b_j f(t_n + c_j h, \vec{k}_j) \\ \vec{y}_{n+1} &= \vec{y}_n + h\sum_{j=1}^{v} b_j f(t_n + c_j h, \vec{k}_j) \end{aligned}\right\} \text{Explicit}$$

$$\begin{array}{c|cccc} c_1 & & & & \\ c_2 & a_{2,1} & & & \\ c_3 & a_{3,1} & a_{3,2} & & \\ \vdots & & & & \\ c_v & a_{v,1} & a_{v,2} & \cdots & a_{v,v-1} \\ \hline & b_1 & b_2 & b_{v-1} & b_v \end{array}$$

A is lower triangular

Explicit

Implicit:
$$\begin{array}{c|ccc} c_1 & a_{1,1} & \cdots & a_{1,\nu} \\ \vdots & \vdots & \ddots & \vdots \\ c_\nu & a_{\nu,1} & \cdots & a_{\nu,\nu} \\ \hline & b_1 & \cdots & b_\nu \end{array}$$

Example 2-stage IRK

$$\vec{k}_1 = \vec{y}_n + h\sum_{i=1}^{2} a_{1,i}\vec{f}(t_n + c_i h, \vec{k}_2)$$

$$\vec{k}_2 = \vec{y}_n + h\sum_{i=1}^{2} a_{2,i}\vec{f}(t_n + c_i h, \vec{k}_2)$$

$$\Longrightarrow \begin{bmatrix} \vec{k}_1 \\ \vec{k}_2 \end{bmatrix} = \begin{bmatrix} \tilde{g}_1(\vec{k}) \\ \tilde{g}_2(\vec{k}) \end{bmatrix}$$

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ERK
- $\sum_{i=1}^{\nu-1} a_{j,i} = c_j$, $j=1,\dots,\nu$
- other constraints on a_i's, b_i's, c_i's result in higher order RK (Taylor, p.3)

IRK
- $\sum_{i=1}^{\nu} a_{j,i} = c_j$
- to obtain higher order RK we do not use Taylor, but we consider collocation methods (§3.4)

Where does $\sum_{i=1}^{\nu} a_{j,i} = c_i$ come from? Let's look at IRK for

$$\vec{y}\,'(t) = \vec{f}(t, \vec{y}(t)),\quad \vec{y}(t_n) = \vec{y}_n$$

$$k_j = \vec{y}_n + h\sum_{i=1}^{\nu} a_{j,i}\vec{f}(t_n + c_i h, \vec{k}_i)$$

$$\vec{y}_{n+1} = \vec{y}_n + h\sum_{j=1}^{\nu} b_j \vec{f}(t_n + c_j h, \vec{k}_j)$$

The IRK for $t' = 1$, $t(0) = t_n$.

$$\tau_j = t_n + h\sum_{i=1}^{\nu} a_{j,i}\cdot 1$$

$$t_{n+1} = t_n + h\sum_{j=1}^{\nu} b_j \cdot 1$$

To develop higher-order IRK methods we need to understand collocation methods

- Choose ν distinct paramaters in $[0,1]$, $c_1, c_2, \ldots, c_\nu$
- Find a ν^{th}-degree polynomial $\vec{u}$ such that

$$\vec{u}(t_n) = \vec{y}_n$$
$$\vec{u}'(t_n + c_j h) = \vec{f}(t_n + c_j h, \vec{u}(t_n + c_j h)), \quad j = 1, 2, \ldots \nu$$

We are solving

$$\vec{y}'(t) = \vec{f}(t, \vec{y}(t)), \quad t \geq t_0, \quad \vec{y}(t_0) = \vec{y}_0$$

- $\vec{u}$ satisfies the initial condition
- $\vec{u}$ satisfies the ODE exactly at ν distinct points $t_n + c_j h$, $j = 1, \ldots, \nu$
- The <u>collocation method</u> consists of finding this $\vec{u}$ and setting

$$\vec{y}_{n+1} := \vec{u}(t_{n+1})$$

- The collocation method is an IRK.

Lemma 3.5: The collocation method is an IRK method with

$$\begin{array}{c|c} \vec{c} & A \\ \hline & \vec{b}^T \end{array}$$

where

$$a_{j,i} = \int_0^{c_j} \frac{q_i(\tau)}{q_i(c_i)} \, d\tau \quad \text{and} \quad b_j = \int_0^1 \frac{q_j(\tau)}{q_j(c_j)} \, d\tau$$

where

$$q(\tau) = \prod_{j=1}^{\nu} (t - c_j) \quad \text{and} \quad q_i(t) = \frac{q(t)}{t - c_i}.$$

Proof: Define Lagrange interpolation polynomials

$$\vec{r}(t) = \sum_{\ell=1}^{\nu} \frac{q_\ell\left(\frac{t - t_n}{h}\right)}{q_\ell(c_\ell)} \vec{\omega}_\ell.$$

Then

$$\vec{r}(t_n + c_j h) = \sum_{\ell=1}^{\nu} \frac{q_\ell(c_j)}{q_\ell(c_\ell)} \vec{\omega}_\ell = \vec{\omega}_j.$$

Choose $\vec{\omega}_\ell = \vec{u}'(t_n + c_\ell h)$.

$\vec{u}$ is a polynomial of degree ν, $\vec{u}'$ is a polynomial of degree $\nu - 1$, and $\vec{r}$ is a polynomial of degree $\nu - 1$. Since $\vec{r}$ and $\vec{u}'$ coincide at ν points, we conclude that $\vec{r} = \vec{u}'$. Therefore

$$\vec{u}'(t) = r(t) = \sum_{\ell=1}^{\nu} \frac{q_\ell((t - t_n)/h)}{q_\ell(c_\ell)} \vec{u}'(t_n + c_\ell h)$$

$$= \sum_{\ell=1}^{\nu} \frac{q_\ell((t-t_n)/h)}{q_\ell(c_\ell)} \vec f(t_n+c_\ell h, \vec u(t_n+c_\ell h)).$$

Integrate from t_n to t:

$$\vec u(t) = \vec u(t_n) + \int_{t_n}^{t} \sum_{\ell=1}^{\nu} \frac{q_\ell((t-t_n)/h)}{q_\ell(c_\ell)} \vec f(t_n+c_\ell h, \vec u(t_n+c_\ell h))\,dt$$

$$= \vec y_n + h\sum_{\ell=1}^{\nu} \vec f(t_n+c_\ell h, \vec u(t_n+c_\ell h)) \int_0^{(t-t_n)/h} \frac{q_\ell(\tau)}{q_\ell(c_\ell)}\, d\tau \qquad \tau = \frac{t-t_n}{h}$$

Set $\vec k_j = \vec u(t_n+c_j h)$, $j=1,2,\dots,\nu$. Then

$$\vec k_j = \vec y_n + h\sum_{i=1}^{\nu} a_{j,i}\vec f(t_n+c_\ell h, \vec k_i)$$

where

$$a_{j,i} = \int_0^{c_j} \frac{q_i(\tau)}{q_i(c_i)}\, d\tau.$$

Also

$$\vec y_{n+1} = \vec u(t_{n+1}) = \vec y_n + h\sum_{j=1}^{\nu} b_j \vec f(t_n+c_j h, \vec k_j)$$

where

$$b_j = \int_0^{1} \frac{q_j(\tau)}{q_j(c_j)}\, d\tau.$$

- Collocation methods are IRK methods
- __Not__ every IRK method is a collocation

Difference between __error__ and __defect__: Consider the ODE

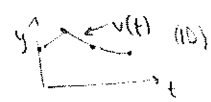
$$\vec y\,'(t) = \vec f(t, \vec y(t)),\ t \geq t_0,\ \vec y(t_0) = \vec y_0.$$

Assume we have found an approximate solution

$$\vec y_0, \vec y_1, \vec y_2, \dots, \vec y_N.$$

By interpolation we can extend this "grid" function to the whole domain, $\vec v(t)$

The defect is defined as



$$\vec d(t) = \vec v\,'(t) - \vec f(t, \vec v(t)),$$

and the error is defined as

$$\vec e(t) = \vec v(t) - \vec y(t).$$

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<u>Example</u> Linear ODE $\vec{y}\,'(t) = A\vec{y}(t)$, $\vec{y}(t_0) = \vec{y}_0$

The defect is $\vec{d}(t) = \vec{v}\,'(t) - A\vec{v}(t)$. Rewrite defect as $\vec{v}\,'(t) = A\vec{v}(t) + \vec{d}(t)$, $t \geq t_0$, $\vec{v}(t_0)$ given. The exact solution to "defect" ODE:

$$\vec{v}(t) = \exp((t-t_0)A)\vec{v}_0 + \int_{t_0}^{t} \exp((t-\tau)A)\vec{d}(\tau)\,d\tau$$

The exact solution to ODE:

$$\vec{y}(t) = \exp((t-t_0)A)\vec{y}_0$$

The error can be written in terms of known data only:

$$\vec{e}(t) = \vec{v}(t) - \vec{y}(t) = \exp((t-t_0)A)(\vec{v}_0 - \vec{y}_0) + \int_{t_0}^{t} \exp((t-\tau)A)\vec{d}(\tau)\,d\tau .$$

Theorem 3.6: Let $\vec{v}(t)$ be such that $\vec{v}(t_0) = \vec{y}(t_0)$ where y solves $\vec{y}\,'(t) = \vec{f}(t, \vec{y}(t))$. Then

proof omitted

defect: $\vec{f}(\tau, \vec{v}(\tau)) - \vec{v}\,'(\tau)$

$$\vec{e}(t) = \int_{t_0}^{t} \Phi(t, \tau, \vec{v}(\tau))\vec{d}(\tau)\,d\tau$$

negative of previous definition

where Φ is a matrix $\frac{\partial \vec{\omega}}{\partial \vec{v}(\tau)}$ where $\vec{\omega}$ is the solution of $\vec{\omega}\,' = \vec{f}(t, \vec{\omega})$ with initial condition $\vec{\omega}(\tau) = \vec{v}(\tau)$.

Theorem 3.7: Suppose

$$\int_0^1 q(\tau)\tau^j\,d\tau = 0, \quad j = 0, 1, \ \ , m-1$$

for $m \in \{0, 1, 2, \ldots, \nu\}$, where recall

$$q(\tau) = \prod_{\ell=1}^{\nu}(t - c_\ell).$$

Then the collocation method is order $\nu + m$.

Proof: Collocation method: find a ν^{th}-degree polynomial $\vec{u}$ such that $\vec{u}(t_n) = \vec{y}_n$ and $\vec{u}\,'(t_n + c_j h) = \vec{f}(t_n + c_j h, \vec{u}(t_n + c_j h))$. Then $\vec{y}_{n+1} = \vec{u}(t_{n+1})$.

Let $\tilde{y}$ be the exact solution to $\tilde{y}\,'(t) = \vec{f}(t, \tilde{y}(t))$, $\tilde{y}(t_n) = t_n$.

The error at $t = t_{n+1}$ is given by

$$\vec{y}_{n+1} - \tilde{y}(t_{n+1}) = \vec{u}(t_{n+1}) - \tilde{y}(t_{n+1}) = \int_{t_n}^{t_{n+1}} \Phi(t_{n+1}, \tau, \vec{u}(\tau))\vec{d}(\tau)\,d\tau .$$

For the integral, we use the quadrature formula with respect to the weight function $\omega(t)=1$, with nodes $t_n+c_1h, \dots, t_n+c_\nu h$. Then

$$\tilde{y}_{n+1}-\hat{y}_{n+1}=\sum_{j=1}^{\nu} b_j \Phi(t_{n+1}, t_n+c_jh, \vec{u}(t_n+c_jh))\vec{d}(t_n+c_jh) + \text{error of quadrature.}$$

However note that

$$\vec{d}(t_n+c_jh)=\vec{u}'(t_n+c_jh)-\vec{f}(t_n+c_jh, \vec{u}(t_n+c_jh))=0.$$

So

$$\tilde{y}_{n+1}-\hat{y}_{n+1} = \text{error of quadrature formula.}$$

By theorem 3.4, if we let $r\in\mathbb{P}_\nu$ such that $\langle r, \hat{p}\rangle=0 \ \forall \hat{p}\in\mathbb{P}_{m-1}$, $\langle r, t^m\rangle \neq 0$, and $c_1, c_2, \dots c_\nu$ are the zero's of r, then the quadrature formula is order $\nu+m$.

We will look at the polynomial $q(t)$:

$$\langle q, \tau^j\rangle = \int_0^1 q(\tau)\tau^j d\tau = \int_0^1 \underbrace{\prod_{\ell=1}^{\nu}(t-c_\nu)}_{\mathbb{P}_\nu} \underbrace{\tau^j}_{\mathbb{P}_j} d\tau = 0 \quad \text{for } j=0, \dots, m-1 \text{ for } m\in\{0,1,\dots,\nu\}$$

we want this?

So, with $g(\tau)=q(\tau)\tau^j$,

$$\int_0^1 q(\tau)\tau^j d\tau = \sum_{j=1}^{\nu} b_j g(c_j) + \alpha g^{(p+m)}(\eta), \quad \eta\in[0,1].$$

Change of variables: $t=t_n+h\tau$. Then, with $\hat{g}(t)=g(\tau)$,

$$\frac{d^{p+m}g(\tau)}{d\tau^{p+m}} = h^{p+m}\frac{d^{p+m}\hat{g}(t)}{dt^{p+m}}.$$

$$\int_0^1 g(\tau)d\tau = \frac{1}{h}\int_{t_n}^{t_{n+1}} \hat{g}(t)dt$$

$$\Rightarrow \frac{1}{h}\int_{t_n}^{t_{n+1}}\hat{g}(t)dt = \sum_{j=1}^{\nu}\hat{g}(t_n+c_jh)b_j + \alpha h^{p+m}\frac{d^{p+m}\hat{g}}{dt^{p+m}} \rightarrow \int_{t_n}^{t_{n+1}} g(t)dt = \Sigma \cdots + O(h^{\nu+m+1}). \blacksquare$$

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If $c_1, c_2, \dots, c_\nu$ are zeros of a polynomial $\tilde{P}_\nu\in\mathbb{P}_\nu$ that is orthogonal with respect to $\omega(t)=1$, then the collocation method is of order 2ν.

$$\int_0^1 q(\tau)\tau^j d\tau = \langle q(\tau), \tau^j\rangle = 0 \quad \text{for } j\leq \nu-1.$$

Gauss-Legendre Runge-Kutta methods

$c_1, c_2, \dots, c_\nu$ are zeros of polynomials $\tilde{P}_\nu\in\mathbb{P}_\nu$ that are orthogonal with respect to weight $\omega(\tau)=1$. These polynomials are the Legendre polynomials transformed to $[0,1]$:

$$\hat{P}_\nu(t) = \frac{(\nu!)^2}{(2\nu)!}\sum_{k=0}^{\nu}(-1)^{\nu-k}\binom{\nu}{k}\binom{\nu+k}{k}t^k.$$

A 1-stage 2nd order IRK method:

$$\hat{P}_1(t) = \frac{(1!)^2}{2!}\left((-1)^{1-0}\binom{1}{0}\binom{1}{0}t^0 + (-1)^{1-1}\binom{1}{1}\binom{2}{1}t\right) = t - \frac{1}{2}$$

$$\longrightarrow c_1 = \frac{1}{2}$$

Use lemma 3.5 to get

$$a_{11} = \int_0^{c_1} 1\,d\tau = c_1, \qquad b_1 = \int_0^1 1\,d\tau = 1$$

Butcher tableau: $\begin{array}{c|c} \frac{1}{2} & \frac{1}{2} \\ \hline & 1 \end{array}$

$$\vec{k}_1 = \vec{y}_n + \tfrac{1}{2}h\vec{f}(t_n + \tfrac{1}{2}h, \vec{k}_1)$$
$$\vec{y}_{n+1} = \vec{y}_n + h\vec{f}(t_n + \tfrac{1}{2}h, \vec{k}_1)$$

We can eliminate $\vec{k}_1$ to simplify this method

$$\vec{k}_1 - \vec{y}_{n+1} = \vec{y}_n + \tfrac{1}{2}h\vec{f}(t_n+\tfrac{1}{2}h, \vec{k}_1) - \tfrac{1}{2}\vec{y}_n - \tfrac{1}{2}\cancel{h\vec{f}(t_n+\tfrac{1}{2}h, \vec{k}_1)}$$
$$\Longrightarrow \vec{k}_1 = \tfrac{1}{2}(\vec{y}_n + \vec{y}_{n+1})$$

So

$$\vec{y}_{n+1} = \vec{y}_n + h\vec{f}(t_n + \tfrac{1}{2}h,\ \tfrac{1}{2}(\vec{y}_n + \vec{y}_{n+1})).$$

Example: A 2-stage 4th order IRK method.

$$\hat{P}_2(t) = \frac{(2!)^2}{4!}\left((-1)^2\binom{2}{0}\binom{2}{0}t^0 + (-1)^1\binom{2}{1}\binom{3}{1}t^1 + (-1)^0\binom{2}{2}\binom{4}{2}t^2\right)$$
$$= \frac{1}{6} - t + t^2$$

$$\rightarrow c_1 = \frac{1}{2} - \frac{1}{6}\sqrt{3}, \quad c_2 = \frac{1}{2} + \frac{1}{6}\sqrt{3}$$

Use lemma 3.5:

$$q(t) = (t-c_1)(t-c_2), \quad q_1(t) = (t-c_2), \quad q_2(t) = (t-c_1)$$

$$a_{11} = \int_0^{c_1}\frac{q_1(t)}{q_1(c_1)}dt = \frac{1}{4}, \quad a_{12} = \frac{1}{4} - \frac{1}{6}\sqrt{3}, \quad a_{21} = \frac{1}{4} + \frac{1}{6}\sqrt{3}, \quad a_{22} = \frac{1}{4}$$

$$b_1 = \int_0^1 \frac{q_1(\tau)}{q_1(c_1)}d\tau = \frac{1}{2}, \quad b_2 = \int_0^1 \frac{q_2(\tau)}{q_2(c_2)}d\tau = \frac{1}{2}$$

$$\begin{array}{c|cc} \frac{1}{2} - \frac{1}{6}\sqrt{3} & \frac{1}{4} & \frac{1}{4} - \frac{1}{6}\sqrt{3} \\ \frac{1}{2} + \frac{1}{6}\sqrt{3} & \frac{1}{4} + \frac{1}{6}\sqrt{3} & \frac{1}{4} \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}$$