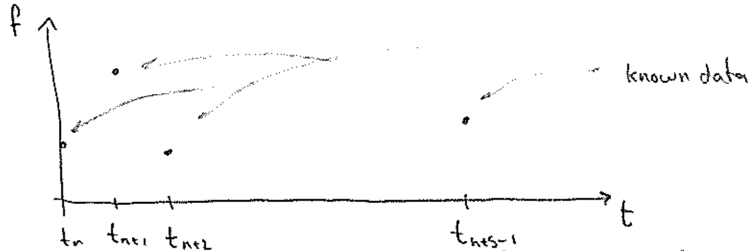
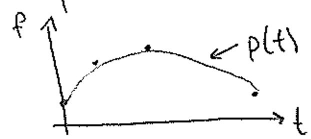
Chapter 2: Multistep Methods

Use $\vec{y}_n, \vec{y}_{n-1}, \vec{y}_{n-2}, \ldots$ to find $\vec{y}_{n+1}$.

- Consider the time interval $[t_{n+s-1}, t_{n+s}]$, assume we have computed $\vec{y}_{n+m}$, $m=0,1,2,\ldots,s-1$. Then we know $\vec{f}(t_{n+m}, \vec{y}_{n+m})$, $m=0,1,2,\ldots,s-1$.



Idea: fit a polynomial $\vec{p}(t)$ that matches $\vec{f}(t_{n+m}, \vec{y}_{n+m})$, $m=0,1,2,\ldots,s-1$



$$\vec{p}(t) = \sum_{m=0}^{s-1} p_m(t)\vec{f}(t_{n+m}, \vec{y}_{n+m})$$

$p_m(t)$ has to satisfy

$$p_m(t_{n+k}) = \begin{cases} 1, & k=m, \\ 0, & k\neq m, \end{cases}$$

$$p_m(t) = \prod_{\substack{l=0 \\ l\neq m}}^{s-1} \frac{t - t_{n+l}}{t_{n+m} - t_{n+l}}$$

Lagrange interpolation polynomials

$$p_m(t_{n+m}) = \prod_{\substack{l=0 \\ l\neq m}}^{s-1} \frac{t_{n+m} - t_{n+l}}{t_{n+m} - t_{n+l}} = \prod 1 = 1$$

$k\neq m$: $$p_m(t_{n+k}) = \prod_{\substack{l=0 \\ l\neq m}}^{s-1} \underbrace{\frac{t_{n+k} - t_{n+l}}{t_{n+m} - t_{n+l}}}_{=0 \text{ for } k=l} = 0$$

2016 01 12

Solve

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

restrict to $[t_{n+s-1}, t_{n+s}]$

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

$$\Rightarrow \vec{y}(t_{n+s}) = \vec{y}(t_{n+s-1}) + \int_{t_{n+s-1}}^{t_{n+s}} \vec{f}(t, \vec{y}(t))\,dt$$

Approximate now $\vec{f}(t, \vec{y}(t))$ by polynomial $\vec{p}(t)$

$$\int_{t_{n+s-1}}^{t_{n+s}} \vec{f}(t, \vec{y})\,dt \approx \int_{t_{n+s-1}}^{t_{n+s}} \vec{p}(t)\,dt = \sum_{m=0}^{s-1} \vec{f}(t_{n+m}, \vec{y}_{n+m}) \int_{t_{n+s-1}}^{t_{n+s}} p_m(t)\,dt$$

Define

$$b_m = \frac{1}{h} \int_{t_{n+s-1}}^{t_{n+s}} p_m(t)\,dt = \frac{1}{h} \int_0^h p_m(t_{n+s-1} + \tau)\,d\tau \qquad (\tau = t - t_{n+s-1})$$

$$\Rightarrow \int_{t_{n+s-1}}^{t_{n+s}} \vec{f}(t, \vec{y}(t))\,dt \approx h \sum_{m=0}^{s-1} b_m \vec{f}(t_{n+m}, \vec{y}_{n+m})$$

Our first multistep method:

$$\vec{y}_{n+s} = \vec{y}_{n+s-1} + h \sum_{m=0}^{s-1} b_m \vec{f}(t_{n+m}, \vec{y}_{n+m})$$

(Adams-Bashforth methods)

<u>Examples</u>

<u>s=1</u>: $\vec{y}_{n+1} = \vec{y}_n + h b_0 \vec{f}(t_n, \vec{y}_n)$

$$b_0 = \frac{1}{h} \int_0^h p_0(t_n + \tau)\,d\tau = 1 \quad \text{as } p_0(t) = 1$$

<u>s=2</u>: $\vec{y}_{n+2} = \vec{y}_{n+1} + h b_0 \vec{f}(t_n, \vec{y}_n) + h b_1 \vec{f}(t_{n+1}, \vec{y}_{n+1})$

$$p_m(t) = \prod_{\substack{\ell=0 \\ \ell \neq m}}^{s-1} \frac{t - t_{n+\ell}}{t_{n+m} - t_{n+\ell}} = \begin{cases} \dfrac{t - t_{n+1}}{t_n - t_{n+1}}, & m = 0 \\[2ex] \dfrac{t - t_n}{t_{n+1} - t_n}, & m = 1 \end{cases}$$

$$b_0 = \frac{1}{h} \int_0^h p_0(t_{n+1} + \tau)\,d\tau = \frac{1}{h} \int_0^h \frac{t_{n+1} + \tau - t_{n+1}}{t_n - t_{n+1}}\,d\tau = -\frac{1}{h^2} \int_0^h \tau\,d\tau = -\frac{1}{2}$$

$$b_1 = \frac{1}{h} \int_0^h p_1(t_{n+1} + \tau)\,d\tau = \frac{1}{h} \int_0^h \frac{t_{n+1} + \tau - t_n}{t_{n+1} - t_n}\,d\tau = \frac{1}{h} \int_0^h \frac{h + \tau}{h}\,d\tau = \frac{3}{2}$$

$$\vec{y}_{n+2} = \vec{y}_{n+1} + h\left(-\frac{1}{2} \vec{f}(t_n, \vec{y}_n) + \frac{3}{2} \vec{f}(t_{n+1}, \vec{y}_{n+1})\right)$$

The s-step method is of order s (proof later). $\Rightarrow$ by halving h the global error decays as $O(h^s)$.

s=1: halve h → global error decrease by a factor of 2
s=2: halve h → global error decrease by a factor of 4
s=3: halve h → global error decrease by a factor of 8
s=n: halve h → global error decrease by a factor of 2^n

§2.2: Order and convergence of multistep methods

General s-step method:

$$(*) \quad \sum_{m=0}^{s} a_m \vec{y}_{n+m} = h \sum_{m=0}^{s} b_m \vec{f}(t_{n+m}, \vec{y}_{n+m}), \quad n=0,1,2,3,\ldots$$

- a_m, b_m are constants independent of h and n
- $b_s = 0 \longrightarrow$ Explicit method

  $b_s \neq 0 \longrightarrow$ Implicit method

Question: how do we choose a_m and b_m?
→ Choose a_m, b_m such that the order of the method is reasonable.

By definition, the order of s-step method is order p if and only if

$$\vec{\psi}(t,\vec{y}) = \sum_{m=0}^{s} a_m \vec{y}(t+mh) - h\sum_{m=0}^{s} b_m \vec{f}(t+mh, \vec{y}(t+mh))$$
$$= \sum_{m=0}^{s} a_m \vec{y}(t+mh) - h\sum_{m=0}^{s} b_m \vec{y}'(t+mh)$$
$$= \mathcal{O}(h^{p+1}).$$

Define

$$\rho(w) = \sum_{m=0}^{s} a_m w^m, \quad \sigma(w) = \sum_{m=0}^{s} b_m w^m$$

Thm 2.1 The multistep method $(*)$ is of order $p \geq 1$ if and only if there is a $c \neq 0$ such that

$$\rho(w) - \sigma(w)\ln(w) = c(w-1)^{p+1} + \mathcal{O}(|w-1|^{p+2}), \quad w \to 1$$

Proof:

$$\vec{\psi}(t,\vec{y}) = \sum_{m=0}^{s} a_m \vec{y}(t+mh) - h\sum_{m=0}^{s} b_m \vec{y}'(t+mh)$$

Taylor series expansion around t:

$$\vec{y}(t+mh) = \sum_{k=0}^{\infty} \frac{1}{k!} \vec{y}^{(k)} (mh)^k$$

$$\vec{y}'(t+mh) = \sum_{k=0}^{\infty} \frac{1}{k!} \vec{y}^{(k+1)} (mh)^k$$

So

$$\vec{\Psi}(t,\vec{y}) = \sum_{m=0}^{s} a_m \left(\sum_{k=0}^{\infty} \frac{1}{k!} \vec{y}^{(k)} (mh)^k\right) - h \sum_{m=0}^{s} b_m \left(\sum_{m=0}^{s} \frac{1}{k!} \vec{y}^{(k+1)} (mh)^k\right)$$

$$= \underbrace{\sum_{k=0}^{\infty} \sum_{m=0}^{s} a_m \frac{1}{k!} \vec{y}^{(k)} (mh)^k}_{} - \underbrace{\sum_{k=0}^{\infty} \sum_{m=0}^{s} h b_m \frac{1}{k!} \vec{y}^{(k+1)} (mh)^k}_{}$$

$$\left(\sum_{m=0}^{s} a_m\right) \vec{y}(t) + \sum_{k=1}^{\infty} \frac{1}{k!} \left(\sum_{m=0}^{s} m^k a_m\right) h^k \vec{y}^{(k)} \quad \underbrace{\sum_{k=1}^{\infty} \sum_{m=0}^{s} b_m \frac{1}{(k-1)!} \vec{y}^{(k)} m^{k-1} h^k}_{}$$

$$\sum_{k=1}^{\infty} \frac{1}{k!} \left(k \sum_{m=0}^{s} m^{k-1} b_m\right) h^k \vec{y}^{(k)}$$

$$\vec{\Psi}(t,\vec{y}) = \left(\sum_{m=0}^{s} a_m\right) \vec{y}(t) + \sum_{k=1}^{\infty} \frac{1}{k!} \left(\sum_{m=0}^{s} m^k a_m - k \sum_{m=0}^{s} m^{k-1} b_m\right) h^k \vec{y}^{(k)}(t)$$

For this method to be order p we need

$$\sum_{m=0}^{s} a_m = 0 \quad \text{and} \quad \sum_{m=0}^{s} m^k a_m = k \sum_{m=0}^{s} m^{k-1} b_m \quad \text{for } k = 1, 2, \dots, p$$

$$\text{and} \quad \sum_{m=0}^{s} m^k a_m \neq k \sum_{m=0}^{s} m^{k-1} b_m \quad \text{if} \quad k = p+1$$

$\Rightarrow$ gives conditions for a_m and b_m.

We will use these conditions on a_m and b_m to prove the theorem. 2016 01 14

$$\rho(w) - \sigma(w)\ln(w) \overset{w=\exp(z)}{=} \rho(e^z) - z\sigma(e^z)$$

$$= \sum_{m=0}^{s} a_m e^{mz} - z \sum_{m=0}^{s} b_m e^{mz}$$

$$= \sum_{m=0}^{s} a_m \left(\sum_{k=0}^{\infty} \frac{1}{k!} m^k z^k\right) - z \sum_{m=0}^{s} b_m \left(\sum_{k=0}^{\infty} \frac{1}{k!} m^k z^k\right)$$

$$= \underbrace{\sum_{k=0}^{\infty} \frac{1}{k!} \left(\sum_{m=0}^{s} a_m m^k\right) z^k}_{} - \underbrace{\sum_{k=0}^{\infty} \frac{1}{k!} \left(\sum_{m=0}^{s} m^k b_m\right) z^{k+1}}_{}$$

$$\cancelto{0}{\left(\sum_{m=0}^{s} a_m\right)} + \sum_{k=1}^{\infty} \frac{1}{k!} \left(\sum_{m=0}^{s} a_m m^k\right) z^k \qquad \sum_{k=1}^{\infty} \frac{1}{(k-1)!} \left(\sum_{m=0}^{s} m^{k-1} b_m\right) z^k$$

Using conditions on a_m and b_m

$$\rho(e^z) - z\sigma(e^z) = Cz^{p+1} + \underbrace{\sum_{k=p+2}^{\infty} \frac{1}{k!}\left(\sum_{m=0}^{s} a_m m^k - k\sum_{m=0}^{s} m^{k-1} b_m\right) z^k}_{\mathcal{O}(z^{p+2})}$$

Restore $w = e^z$

$$\begin{aligned}\rho(w) - \ln(w)\sigma(w) &= C(\ln(w))^{p+1} + \mathcal{O}((\ln(w))^{p+2}) \\ &= C(w-1)^{p+1} + \mathcal{O}(|w-1|^{p+2})\end{aligned}$$

because around $w = 1$ we have

$$h(w) = (w-1) + \mathcal{O}(|w-1|^2).$$

2-step Adams-Bashforth method:

$$\vec{y}_{n+2} = \vec{y}_{n+1} + h\left(\frac{3}{2}\vec{f}(t_{n+1}, \vec{y}_{n+1}) - \frac{1}{2}\vec{f}(t_n, \vec{y}_n)\right)$$

What is the order of this method?

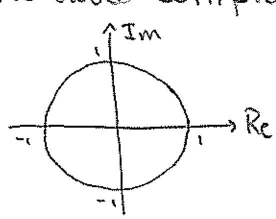
$$\underset{a_0=0}{} \underset{a_1=-1}{-\vec{y}_{n+1}} + \underset{a_2=1}{\vec{y}_{n+2}} = h\left(\underset{b_0=-\frac{1}{2}}{-\frac{1}{2}\vec{f}(t_n,\vec{y}_n)} + \underset{b_1=\frac{3}{2}}{\frac{3}{2}\vec{f}(t_{n+1},\vec{y}_{n+1})}\right)$$

$$\rho(w) = \sum_{m=0}^{s} a_m w^m = -w + w^2, \quad \sigma(w) = \sum_{m=0}^{s} b_m w^m = -\frac{1}{2} + \frac{3}{2}w$$

$$\begin{aligned}\rho(w) - \sigma(w)\ln(w) &\overset{\xi = w-1}{=} \rho(\xi+1) - \sigma(\xi+1)\underbrace{\ln(\xi+1)}_{\xi - \frac{1}{2}\xi^2 + \frac{1}{3}\xi^3 - \frac{1}{4}\xi^4 + \cdots} \\ &= (\xi^2 + \xi) - \left(1 + \frac{3}{2}\xi\right)\left(\xi - \frac{1}{2}\xi^2 + \frac{1}{3}\xi^2 + \cdots\right) \\ &= \frac{5}{12}\xi^3 + \mathcal{O}(\xi^4).\end{aligned}$$

$\Rightarrow p = 2$

A polynomial satisfies the <u>root condition</u> if all of its zeros reside in the closed complex unit disk and all its zeros of unit modulus are simple.



$f(x) = (x-1)(x+1)$ ✓

$f(x) = (x-1)^2$ ×

$f(x) = (x-1)(x-2)x$ ×

Proof omitted

Theorem 2.2 [Dahlquist equivalence theorem]:
Suppose that the error in $\vec{y}_1, \vec{y}_2, \vec{y}_3, \dots, \vec{y}_{s-1}$ tends to zero as $h \to 0$.
Then the multistep method

$$\sum_{m=0}^{s} a_m \vec{y}_{n+m} = h \sum_{m=0}^{s} b_m \vec{f}(t_{n+m}, \vec{y}_{n+m}), \quad n = 0, 1, 2, \dots$$

is convergent if and only if it is of order $p \geq 1$ and

$$\rho(w) = \sum_{m=0}^{s} a_m w^m$$

obeys the root condition.

Example: Is

$$\vec{y}_{n+2} - 3\vec{y}_{n+1} + 2\vec{y}_n = h\left(\frac{13}{12}\vec{f}(t_{n+2}, \vec{y}_{n+2}) - \frac{5}{3}\vec{f}(t_{n+1}, \vec{y}_{n+1}) - \frac{5}{12}\vec{f}(t_n, \vec{y}_n)\right)$$

convergent?
The order of this method is 2. (check just like previous example)

$$\rho(w) = \sum_{m=0}^{2} a_m w^m \quad \text{where } a_0 = 2,\ a_1 = -3,\ a_2 = 1$$

$$\longrightarrow \rho(w) = 2 - 3w + w^2 = (w-1)(w-2)$$

Example Adams-Bashforth methods

$$\vec{y}_{n+s} = \vec{y}_{n+s-1} + h \sum_{m=0}^{s-1} b_m \vec{f}(t_{n+m}, \vec{y}_{n+m})$$

Convergent for $s \geq 1$?
We saw these are of order s.

$$\rho(w) = \sum_{m=0}^{s} a_m w^m \quad \text{where } a_s = 1,\ a_{s-1} = -1,\ a_k = 0,\ k = 0, 1, 2, \dots, s-2$$

$$\Rightarrow \rho(w) = w^s - w^{s-1} = w^{s-1}(w-1)$$

The maximum order that an s-step method can achieve is

$$p = \begin{cases} 2\left\lfloor \frac{s+2}{2} \right\rfloor, & \text{implicit} \\ s, & \text{explicit} \end{cases}$$

In practice, you want to construct s-step methods of order

$$p = \begin{cases} s+1, & \text{implicit} \\ s, & \text{explicit} \end{cases}$$

2016 01 18

Use $\rho(\omega)$ and $\sigma(\omega)$ to develop new multistep methods.

Step 1: Choose an arbitrary polynomial $\rho(\omega)$ of degree s that obeys the root condition and such that $\rho(1)=0$

↳ convergence ↳ Thm 2.1, to ensure method is of order at least 1

Step 2: Theorem 2.1 states that method is of order $p \geq 1$ if and only if

$$\rho(\omega) - \sigma(\omega)\ln(\omega) = c(\omega-1)^{p+1} + \mathcal{O}(|\omega-1|^{p+2})$$

$$= \mathcal{O}(|\omega-1|^{p+1})$$

$$\Rightarrow \sigma(\omega) = \frac{\rho(\omega)}{\ln(\omega)} + \mathcal{O}(|\omega-1|^{p}).$$

Step 3: Expand $\frac{\rho(\omega)}{\ln(\omega)}$ in a Taylor series around $\omega = 1$.

Step 4: Decide whether you want an explicit method or an implicit method.

Step 5: Implicit method: Take $\sigma(\omega)$ as s^{th}-degree polynomial that matches the Taylor series of $\frac{\rho(\omega)}{\ln(\omega)}$ up to $\mathcal{O}(|\omega-1|^{s+1})$.

Explicit method: Take $\sigma(\omega)$ as $(s-1)^{th}$-degree polynomial (so that $b_s = 0$) that matches Taylor series up to $\mathcal{O}(|\omega-1|^{s})$.

Example: Alternative derivation to the 2-step Adams-Bashforth method.

Step 1: $\rho(\omega) = \omega^2 - \omega$

Step 2+3+4: We have a $\rho(\omega)$ → how to find $\sigma(\omega)$? Taylor series expansion of

$$\frac{\rho(\omega)}{\ln(\omega)} = \frac{\omega(\omega-1)}{\ln(\omega)} \overset{\omega=\xi+1}{=} \frac{\xi+\xi^2}{\ln(\xi+1)}$$

$$= (\xi+\xi^2)\left(\frac{1}{\xi} + \frac{1}{2} - \frac{\xi}{12} + \mathcal{O}(\xi^2)\right)$$

$$= 1 + \frac{3}{2}\xi + \frac{5}{12}\xi^2 + \mathcal{O}(\xi^3)$$

because

$$\frac{1}{\ln(\xi+1)} = \frac{1}{\xi} + \frac{1}{2} - \frac{\xi}{12} + \mathcal{O}(\xi^2).$$

For an explicit method, truncate after the linear term:

$$\sigma(w) = 1 + \frac{3}{2}\xi = 1 + \frac{3}{2}(w-1) = -\frac{1}{2} + \frac{3}{2}w$$

Now

$$\rho(w) = -w + w^2 \longrightarrow a_0 = 0,\ a_1 = -1,\ a_2 = 1$$
$$\sigma(w) = -\frac{1}{2} + \frac{3}{2}w \longrightarrow b_0 = -\frac{1}{2},\ b_1 = \frac{3}{2},\ b_2 = 0$$

$$\Rightarrow \vec{y}_{n+2} = \vec{y}_{n+1} + h\left(-\frac{1}{2}\vec{f}(t_n, \vec{y}_n) + \frac{3}{2}\vec{f}(t_{n+1}, \vec{y}_{n+1})\right)$$

For an implicit method, truncate after the quadratic term:

$$\sigma(w) = 1 + \frac{3}{2}\xi + \frac{5}{12}\xi^2 = 1 + \frac{3}{2}(w-1) + \frac{5}{12}(w-1)^2 = -\frac{1}{12} + \frac{2}{3}w + \frac{5}{12}w^2$$

$$\longrightarrow b_0 = -\frac{1}{12},\ b_1 = \frac{2}{3},\ b_2 = \frac{5}{12}$$
$$a_0 = 0,\ a_1 = -1,\ a_2 = 1$$

$$\Rightarrow \vec{y}_{n+2} = \vec{y}_{n+1} + h\left(-\frac{1}{12}\vec{f}(t_n, \vec{y}_n) + \frac{2}{3}\vec{f}(t_{n+1}, \vec{y}_{n+1}) + \frac{5}{12}\vec{f}(t_{n+2}, \vec{y}_{n+2})\right)$$

Well known choices for $\rho(w)$:

1) $\rho(w) = w^{s-1}(w-1) \rightarrow$ s-step Adams-Bashforth (explicit)
s-step Adams-Moulton (implicit) ?

2) $\rho(w) = w^{s-2}(w^2-1) \rightarrow$ explicit Nysrom methods
implicit Milne methods

One other important family of multistep methods:

$$\sigma(w) = \beta w^s \quad \text{for } \beta \in \mathbb{R}\setminus\{0\}$$

$\Rightarrow$ s-order s-step Backward Differentiation Formulae (BDF)

What is $\rho(w)$ for BDF methods? We want the method to be of order s, so:

$$\rho(w) - \ln(w)\sigma(w) = O(|w-1|^{s+1}),\quad w \to 1$$
$$\Rightarrow \rho(w) = \beta w^s \ln(w) + O(|w-1|^{s+1})$$

let $v = w^{-1}$:

$$v^s \rho(v^{-1}) = -\beta \ln(v) + O(|v-1|^{s+1})$$

Taylor series expansion of $\ln(w)$:

$$\ln(v) = \ln(1 + (v-1)) = \sum_{m=0}^{s} \frac{(-1)^{m-1}}{m}(v-1)^m + O(|v-1|^{s+1})$$

$$v^s \rho(v^{-1}) = \beta \sum_{m=1}^{s} \frac{(-1)^m}{m} (v-1)^m + O(|v-1|^{s+1})$$

$$\Rightarrow \quad \sigma(w) = \beta v^{-s} \sum_{m=1}^{s} \frac{(-1)^m}{m} (v-1)^m$$

$$= \beta \sum_{m=1}^{s} \frac{(-1)^m}{m} w^s (w^{-1}-1)^m$$

$$= \beta \sum_{m=1}^{s} \frac{1}{m} w^{s-m} (-w)^m (w^{-1}-1)^m$$

$$= \beta \sum_{m=1}^{s} \frac{1}{m} w^{s-m} (w-1)^m.$$

What about β? We choose β such that $a_s = 1$.

$$\beta \sum_{m=1}^{s} \frac{1}{m} w^{s-m} (w-1)^m = \beta w^{s-1}(w-1) + \beta \frac{1}{2} w^{s-2}(w-1)^2 + \beta \frac{1}{3} m^{s-3} (w-1)^3 + \cdots$$

$$= \underbrace{\beta\left(1 + \tfrac{1}{2} + \tfrac{1}{3} + \tfrac{1}{4} + \cdots\right)}_{a_s} w^s + \cdots$$

$$\Rightarrow \quad \beta = \left(\sum_{m=1}^{s} \frac{1}{m} \right)^{-1}$$