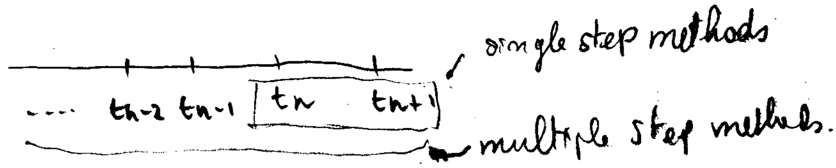
5.6 Multistep methods

Taylor series, Runge Kutta } Single step methods: don't use previous iterations



$$\begin{cases} y' = f(t,y), \ t \in [a,b] \\ y(a) = \alpha \end{cases}$$

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

$$\Rightarrow \boxed{y(t_{n+1}) = y(t_n) + \int_{t_n}^{t_{n+1}} f(t, y(t))\,dt}$$

Idea: use numerical quadrature to approximate integral.

Adams - Bashforth Formula

when formula is of type:

$$y_{n+1} = y_n + a f_n + b f_{n-1} + c f_{n-2} + \cdots$$

where $f_i = f(t_i, y_i)$

Example: Adams - Bashforth formula of order 5 (assumes equally spaced points)

$$y_{n+1} = y_n + \frac{h}{720}\left[1901 f_n - 2774 f_{n-1} + 2616 f_{n-2} - 1274 f_{n-3} + 251 f_{n-4}\right]$$

how to get these coefficients? Using undetermined coeff. method.

$$\int_{t_n}^{t_{n+1}} f(t, y(t))\,dt \approx h\left[A f_n + B f_{n-1} + C f_{n-2} + D f_{n-3} + E f_{n-4}\right]$$

To determine coefficients require that integration formula be exact for all $p \in P_4$ = polynomials with degree ≤ 4.

w.l.o.g. assume $t_n = 0$ and $h = 1$

$$\begin{array}{cccccc} -4 & -3 & -2 & -1 & 0 & 1 \\ t_{n-4} & t_{n-3} & t_{n-2} & t_{n-1} & t_n & t_{n+1} \end{array}$$

Note: it's possible to show that if formula:

$$\int_0^1 f(x)\,dx \approx \sum_{i=-n}^{m} A_i f(i)$$

is exact for $f \in P_m$ then

$$\int_{t_0}^{t_0+h} f(x)\,dx \approx h \sum_{i=-n}^{n} A_i f(t_0+ih)$$

is exact for $f \in P_m$.

A convenient basis for P_4 is then:

$p_0(t) = 1$
$p_1(t) = t$
$p_2(t) = t(t+1)$
$p_3(t) = t(t+1)(t+2)$
$p_4(t) = t(t+1)(t+2)(t+3)$

($\dim P_4 = 5$)

When substituted in the eq:

$$\int_0^1 p_n(t)\,dt = A\,p_n(0) + B\,p_n(-1) + C\,p_n(-2) + D\,p_n(-3) + E\,p_n(-4)$$

$\rightsquigarrow$ get a 5x5 system to solve:

$$\begin{bmatrix} 1 & 1 & 1 & 1 & 1 \\ 0 & -1 & -2 & -3 & -4 \\ 0 & 0 & 2 & 6 & 12 \\ 0 & 0 & 0 & -6 & -24 \\ 0 & 0 & 0 & 0 & 24 \end{bmatrix} \begin{bmatrix} A \\ B \\ C \\ D \\ E \end{bmatrix} = \begin{bmatrix} 1 \\ 1/2 \\ 5/6 \\ 9/4 \\ 251/30 \end{bmatrix}$$

(the basis is chosen in such a way that the system is triangular, and so easy to solve via back substitution)

Adams-Moulton Formula:

Adams Bashforth formulas are often used in conjunction with A-M formulas to get better precision:

$$y_{n+1} = y_n + a f_{n+1} + b f_n + c f_{n-1} + \dots$$

Example: Adams-Moulton formula of order 5

$$(*) \quad y_{n+1} = y_n + \frac{h}{720}\left[251 f_{n+1} + 646 f_n - 264 f_{n-1} + 106 f_{n-2} - 19 f_{n-3}\right]$$

Derivation: similar by method of undetermined coeff.

⚠ x_{n+1} occurs on both sides of equation! we cannot use it directly.

- <u>Predictor-corrector method:</u>

  apply Adam-Bashforth of order m $(x_{n+1}^* = x_n + a f_n + b f_{n-1} + \cdots)$
  —— Adam-Moulton —— m $(x_{n+1} = x_n + \tilde{a} f(t_{n+1}, x_{n+1}^*) + \tilde{b} f_n + \cdots)$

however we still need to prime the iterations to compute the first few x_i.
The idea is to use a method of the same order m:
use Runge-Kutta of order m.

(For example with AB of order 5 and AM of order 5 we need to obtain x_1, x_2, x_3 and x_4 (x_0 is given) using RK of order 5.

- One could view AM formula (say $(*)$ for example) as a mapping with fixed point y_{n+1}:

$$\phi(z) = \frac{251}{720} h f(t_{n+1}, z) + \text{all other terms.}$$

use fixed point iteration:

$$z_{k+1} = \phi(z_k) \quad (z \geq 0)$$

which converges assuming say ϕ is a contraction (Lipschitz cont. with $L<1$)
Assuming f is differentiable it is enough to start iterations at some $z_0 \in B_r(\xi)$ (ball of radius r centered at ξ) where

$$\forall z \in B_r(\xi) \quad |\phi'(z)| < 1.$$

$$\phi'(z) = \frac{251}{720} h \frac{\partial f}{\partial z}(t_{n+1}, z)$$

which can be made as small as we want by decreasing step h.

Only one or two steps are required in practice
(<u>note</u>: this means one carry out correction several times)

Analysis of Multistep Methods

The general form of a (linear) multistep method is:

(**) $a_k y_n + a_{k-1} y_{n-1} + \cdots + a_0 y_{n-k} = h[b_k f_n + b_{k-1} f_{n-1} + \cdots + b_0 f_{n-k}]$

This is a k-step method.

$a_k \neq 0$ since we are computing y_n from $y_{n-1} \ldots y_{n-k}$.

$b_k = 0 \Rightarrow$ explicit method (y_n can be computed directly)

$b_k \neq 0 \Rightarrow$ implicit method (y_n appears in RHS)

A multistep method is said to be of order m if it has same accuracy as a Taylor series method of order m.

A more rigorous def. requires us to define a linear functional:

$$Ly = \sum_{i=0}^{k} \left[a_i y(ih) - h b_i y'(ih) \right]$$

(wlog $k = n$ to simplify notation $\Rightarrow$ (**) starts at $t=0$ instead of $t = (n-k)h$)

Think of L as residual of formula (**) and it can be applied to any differentiable y.

For the analysis we assume y is smooth so that L can be represented using Taylor series of y at 0:

$$Ly = d_0 y(0) + d_1 h y'(0) + d_2 h^2 y''(0) + \cdots$$

where the coeff. d_i can be obtained from the def of L and:

$$y(ih) = \sum_{j=0}^{\infty} \frac{(ih)^j}{j!} y^{(j)}(0)$$

$$y'(ih) = \sum_{j=0}^{\infty} \frac{(ih)^j}{j!} y^{(j+1)}(0)$$

Grouping terms:

h^0 terms: $d_0 = \sum_{i=0}^{k} a_i$

h^1 —: $d_1 = \sum_{i=0}^{k} (i a_i - b_i)$

h^2 — $d_2 = \sum_{i=0}^{k} \left(\frac{1}{2} i^2 a_i - i b_i\right)$

$\vdots$

h^j $d_j = \sum_{i=0}^{k} \left(\frac{i^j}{j!} a_i - \frac{i^{(j-1)}}{(j-1)!} b_i \right)$ $(j \geq 1)$

Theorem The following are equivalent.

i/ $d_0 = d_1 = \dots = d_m = 0$

ii/ $Lp = 0 \quad \forall p \in P_m$ (all poly of degree $\leq m$)

iii/ Ly is $O(h^{m+1}) \quad \forall y \in C^{m+1}$

proof:

i ⇒ ii: i) ⇒ $Ly = d_{m+1} h^{m+1} y^{(m+1)}(0) + \dots$

thus if $p \in P_m$, $p^{(j+1)}(0) = 0$. (for all $j \geq m$)

$\Rightarrow \quad Lp = 0$

ii ⇒ iii: Assume ii. If $y \in C^{m+1}$, by Taylor theorem:

$y = p + r$, where $p \in P^m$.

and r is s.t. $r(0) = r'(0) = \dots = r^{(m)}(0) = 0$

(if you're not convinced:

$y(0) = p(0) + r(0) = y(0) + r(0) \Rightarrow r(0) = 0$.

$y'(0) = p'(0) + r'(0) = y'(0) + r'(0) \Rightarrow r'(0) = 0$ etc....)

Thus: $Ly = L(p+r) = Lr = d_0 r(0) + d_1 h r'(0) + \dots + d_m h^m r^{(m)}(0)$
$+ d_{m+1} h^{m+1} r^{(m+1)}(0) + \dots$

$$\Rightarrow Ly = Lr = d_{m+1} h^{m+1} r^{(m+1)}(0) + o(h^{m+1})$$
$$= O(h^{m+1})$$

iii $\Rightarrow$ i: if $Ly = O(h^{m+1})$ then all coeff in lower orders have to vanish

$$\Rightarrow d_0 = d_1 = d_2 = \dots = d_m = 0.$$

Def: The order of a multistep method is the smallest integer m for which $d_{m+1} \neq 0$:

$$d_0 = d_1 = \dots = d_m = 0 \neq d_{m+1}$$

Example: What is the order of the method:

$$y_n - y_{n-2} = \frac{h}{3}(f_n + 4f_{n-1} + f_{n-2})$$

$a_0 = -1 \qquad b_0 = 1/3$
$a_1 = 0 \qquad b_2 = 4/3$
$a_2 = 1 \qquad b_2 = 1/3$

$\Rightarrow$ $d_0 = a_0 + a_1 + a_2 = 0$

$d_1 = -b_0 + (a_1 - b_1) + (2a_2 - b_2) = 0$

$d_2 = (\frac{1}{2}a_1 - b_1) + (2a_2 - 2b_2) = 0$

$d_3 = (\frac{1}{6}a_1 - \frac{1}{2}b_1) + (\frac{4}{3}a_2 - 2b_2) = 0$

$d_4 = (\frac{1}{24}a_1 - \frac{1}{6}b_1) + (\frac{2}{3}a_2 - \frac{4}{3}b_2) = 0$

$d_5 = (\frac{1}{120}a_1 - \frac{1}{24}b_1) + (\frac{4}{15}a_2 - \frac{2}{3}b_2) = -\frac{1}{90}$

$\Rightarrow$ method is order 4.

Thus it would be easy to design a k-step method of order $2k$ by requiring $d_0 = d_1 = d_2 = \dots = d_{2k} = 0$ ($2k+1$ eq)

the number of unknowns is $2k+2$ and it is possible to show this lin system has a non-trivial sol with $a_k \neq 0$.

however not only the order of the method matters but also stability (to be defined later, but essentially means method does not blow up)

It is possible to show that the order of a stable k-step method is at most $k+2$.

§ 5.7 Variable Step-Size multistep methods

Idea: similar to RKF : • estimate local trunc error from two approx that have different trunc error

• change step size to keep local trunc error smaller.

Example:

Adam Bashforth 4-step method (order 4)

$$y(t_{i+1}) = y(t_i) + \frac{h}{24}\left[55 f_i - 59 f_{i-1} + 37 f_{i-2} - 9 f_{i-3}\right] + \frac{251}{720} h^5 y^{(5)}(\mu_i^{(1)})$$

where $\mu_i^{(1)} \in (t_{i-3}, t_{i+1})$

Adam-Moulton 3-step method (order 4)

$$y(t_{i+1}) = y(t_i) + \frac{h}{24}\left(9 f_{i+1} + 19 f_i - 5 f_{i-1} + f_{i-2}\right) - \frac{19}{720} h^5 y^{(5)}(\mu_i^{(2)})$$

(⚠ book typo ?)

where $\mu_i^{(2)} \in (t_{i-2}, t_{i+1})$

Assuming $y^{(5)}(\mu_i^{(1)}) \approx y^{(5)}(\mu_i^{(2)}) \approx y^{(5)}(\mu)$:

and $y_0, y_1, \dots, y_i$ are exact:

$$y(t_{i+1}) - \tilde{y}_{i+1} \approx \frac{251}{720} h^5 y^{(5)}(\mu) \quad \text{(AB LT error)}$$

$$y(t_{i+1}) - y_{i+1} \approx -\frac{19}{720} h^5 y^{(5)}(\mu) \quad \text{(AM LT error)}$$

$$\Rightarrow \quad y_{i+1} - \tilde{y}_{i+1} \approx \frac{251+19}{720} h^5 y^{(5)}(\mu) = \frac{3}{8} h^5 y^{(5)}(\mu)$$

Thus the AM truncaton error $\tau_{i+1}(h)$ can be approx by:

$$\tau_{i+1}(h) = |y_{i+1} - y(t_{i+1})| \approx \frac{19}{720} h^5 |y^{(5)}(\mu)|$$

$$\approx \frac{19}{720} h^5 \frac{8}{3} \frac{|y_{i+1} - \tilde{y}_{i+1}|}{h^5} = \frac{19}{270} |y_{i+1} - \tilde{y}_{i+1}|$$

Now simulate what would hapen with y_{i+1} and $\tilde{y}_{i+1}$ if we had taken a step qh (call $w_{i+1}, \tilde{w}_{i+1}$ the AM and AB iterates w/ new step size).

$$\tau_{i+1}(qh) = |w_{i+1} - y(t_i + qh)|$$

$$= \frac{19}{720} q^5 h^5 |y^{(5)}(\mu)|$$

$$\approx \frac{19}{720} q^5 h^5 \left[\frac{8}{3} \frac{|y_{i+1} - \tilde{y}_{i+1}|}{h^5}\right]$$

$$= \frac{19}{270} q^5 |y_{i+1} - \tilde{y}_{i+1}|$$

Then we may ask that:

$$\tau_{i+1}(qh) < \underbrace{\varepsilon}_{\text{given precision}} \overbrace{qh}^{\text{new step size}}$$

$$\Rightarrow \quad \frac{19}{270} q^5 |y_{i+1} - \tilde{y}_{i+1}| < \varepsilon q h$$

$$\Rightarrow \quad q < \left(\frac{270}{19} \underbrace{\frac{\varepsilon h}{|y_{i+1} - \tilde{y}_{i+1}|}}\right)^{\frac{1}{4}}$$

$$\approx 2 \left(\quad \swarrow \quad \right)^{\frac{1}{4}}$$

Conservative choice: $q = 1.5 \left(\quad \right)^{\frac{1}{4}}$

potential pitfall: the iterate history kept cannot be used anymore with the new step!
Algo needs to be "primed" again every time step size is changed!
$\rightsquigarrow$ can lead to many function evals.

See algo in book. Same structure as RKF.

$$\begin{cases} y' = f(t,y) \\ y(a) = \alpha \end{cases}$$

§ 5.8 Extrapolation methods.

Idea: Apply a Romberg integration like procedure to a carefully chosen numerical method in order to increase accuracy of next step.

Goal: get successively better approx of $y(a+h)$ by using smaller $h_0 = \frac{h}{2}$ and $h_1 = \frac{h}{4}$ (... other smaller subdivisions can be done, but must be even number)

with $h_0 = \frac{h}{2}$:

$$\eta_0 = y_0 = \alpha$$

$$\eta_1 = \eta_0 + h_0 f(a, \eta_0) \quad \text{(Euler)}$$

$$\eta_2 = \eta_0 + 2h_0 f(a+h_0, \eta_1) \quad \text{(Midpoint)}$$

$$y_{11} = \frac{1}{2}\left[\eta_2 + \eta_1 + h_0 f(a+\underbrace{2h_0}_{=h}, \eta_2)\right] \quad \text{(endpoint correction)}$$

we have:

$$y(a+h) = y_{11} + \delta_1 h_0^2 + \delta_2 h_0^4 + \cdots$$

$$= y_{11} + \delta_1 \left(\frac{h}{2}\right)^2 + \delta_2 \left(\frac{h}{2}\right)^4 + \cdots \quad (1)$$

where δ_i do not depend on h.

with $h_1 = \frac{h}{4}$ -

$\eta_0 = y_0 = \alpha$

$\eta_1 = \eta_0 + h_1 f(a, \eta_0)$ (Euler)

for $j = 1 .. 3$

$\quad \eta_{j+1} = \eta_{j-1} + 2h_1 f(a + jh_1, \eta_j)$ (Midpoint)

$y_{21} = \frac{1}{2}[\eta_4 + \eta_3 + h_1 f(a + \underbrace{4h_1}_{h}, \eta_4)$ (End point correction)

we have:

$$y(a+h) = y_{21} + \delta_1 h_1^2 + \delta_2 h_1^4 + \dots$$

$$= y_{21} + \delta_1 \left(\frac{h}{4}\right)^2 + \delta_2 \left(\frac{h}{4}\right)^4 + \dots \qquad (2)$$

which we can use to cancel out $O(h^2)$ terms with (1):

$\frac{4(2) - (1)}{3}$ gives: $O(h^4)$ error:

$$y(a+h) = y_{21} + \frac{1}{3}(y_{21} - y_{11}) + \delta_2 h^4 \cancel{\underbrace{\frac{1}{3}\left(\frac{1}{4} - 1\right)}_{-\frac{21}{64}}} + \dots$$

(4/4^4 - 1/2^4)/3
= -1/64

thus come up with new approx:

$$y_{22} = y_{21} + \frac{1}{3}(y_{21} - y_{11})$$

And do a Tableau: $\left(h_2 = \frac{h}{6}\right)$

$$\begin{array}{lll}
y_{11} = w(t, h_0) & \searrow & \\
y_{21} = w(t, h_1) & \rightarrow y_{22} & \searrow \\
y_{31} = w(t, h_2) & \rightarrow y_{32} & \rightarrow y_{33} \quad \text{etc} \dots \\
\underbrace{\qquad\qquad}_{O(h^2)} & \underbrace{\qquad}_{O(h^4)} & \underbrace{\qquad}_{O(h^6)}
\end{array}$$

see other update formulas in book.