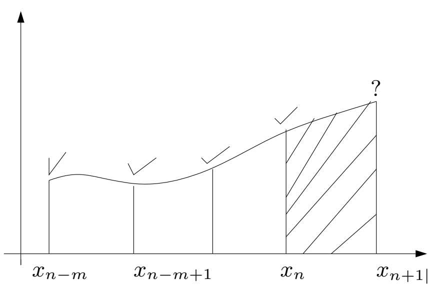
$$
\begin{aligned}
m=1: Y_{n+1} &= Y_n + h\left\{f_n + \frac{1}{2}\Delta f_{n-1}\right\} = Y_n + \frac{h}{2}\{3f_n - f_{n-1}\} && \text{LTE} : O(h^3)\\
m=2: Y_{n+1} &= Y_n + h\left\{f_n + \frac{1}{2}\Delta f_{n-1} + \frac{5}{12}\Delta^2 f_{n-2}\right\}\\
&= Y_n + \frac{h}{12}\{23f_n - 16f_{n-1} + 5f_{n-2}\} && : O(h^4)
\end{aligned}
$$

Note: For an n-step scheme we have n roots. If the method is consistent 1 will be a root. For stability a method has to control the behavior of the remaining $n-1$ roots

- If $|G_j| > 1$ for some j the method is zero-unstable
- If $|G_j| = 1$ for more than one root then the method is weakly zero stable
- This 'useful stability' region in this case is the set of all z such that $|G_j(z)| < 1$ for all j.

A family of implicit multistep methods – Adams Moulton Methods

- By analogy with the trapezoidal scheme we derive a family of methods that use a polynomial to interpolate $f(x, y(x))$ at $x_{n-m}, x_{n-m+1}, \ldots, x_n$ **and** x_{n+1}. Including x_{n+1} makes this family of methods implicit.



Using the interpolation formula derived above

$$f_{n+1+r} = E^r f_{n+1} = \sum_{k=0}^{m+1} (-1)^k \binom{-r}{k} \Delta^k f_{n+1-k}$$

or letting $s = 1 + r$

$$f_{n+s} = E^{(s-1)} f_{n+1} = \sum_{k=0}^{m+1} (-1)^k \binom{1-s}{k} \Delta^k f_{n+1-k}$$

Substituting into the integral form of $y' = f(x, y)$:

$$y_{n+1} = y_n + \int_{x_n}^{x_{n+1}} f(x, y(x))\, dx$$

we obtain

$$
\begin{aligned}
y_{n+1} &= y_n + h\left\{\beta_0 f_{n+1} + \beta_1 \Delta f_n + \ldots + \beta_{m+1}\Delta^{m+1} f_{n-m}\right\}\\
\text{where } \beta_k &= (-1)^k \int_0^1 \binom{1-s}{k}\, ds \qquad k = 0, 1, \ldots, m+1
\end{aligned}
$$

$$\beta_0 = 1, \qquad \beta_1 = -\frac{1}{2} \qquad \beta_2 = -\frac{1}{12}, \qquad \beta_3 = \frac{-1}{24}, \qquad \beta_4 = \frac{-19}{720} \qquad \underline{\text{LTE}}$$

Eg:

$$\begin{aligned}
&\text{AM 1} \quad (m=-1): & Y_{n+1} &= Y_n + hf_{n+1} \quad : \quad \text{Backward Euler} & O(h^2)\\
&\text{AM 2} \quad (m=0): & Y_{n+1} &= Y_n + h\left[f_{n+1} - \frac{1}{2}(f_{n+1}-f_n)\right] = Y_n + \frac{h}{2}[f_{n+1}+f_n]: \ \text{TR} & O(h^3)\\
&\text{AM 3} \quad (m=1): & Y_{n+1} &= Y_n + h\left[f_{n+1} - \frac{1}{2}(f_{n+1}-f_n) - \frac{1}{12}(f_{n+1}-2f_n+f_{n-1})\right] & \\
& & &= Y_n + \frac{h}{12}[5f_{n+1}+8f_n-f_{n-1}] & O(h^4)\\
&\text{AM 4} \quad (m=2): & Y_{n+1} &= Y_n + \frac{h}{24}[9f_{n+1}+19f_n-5f_{n-1}+f_{n-2}] & O(h^5)
\end{aligned}$$

↑ unknown term – need to solve a nonlinear eq.

Stability properties of AM4 – using the perturbation approach.

AM2: $\left(1-\frac{9\lambda h}{24}\right)Y_{n+1} - \left(1+\frac{19\lambda h}{24}\right)Y_n + \frac{5\lambda h}{24}Y_{n-1} - \frac{\lambda h}{24}Y_{n-2} = 0$

Let $r = (\lambda h/24)$

$$(1-9r)Y_{n+1} - (1+19r)Y_n + 5rY_{n-1} - rY_{n-2} = 0$$

Look for solutions of the form $Y_n = G^n$

$$(1-9r)G^3 - (1+19r)G^2 + 5rG - r = 0$$

Now consider the limit $h \ll 1$ so that $r \ll 1$. The $r \to 0$ limit yields the following equation:

$$G_0^3 - G_0^2 = 0$$

which implies that $G_0 = 1, 0, 0$ are the leading terms in the asymptotic expansion for G. Separating the small from the large terms we have

$$G^2(G-1) = r\left\{1 - 5G + 19G^2 + 9G^3\right\}$$

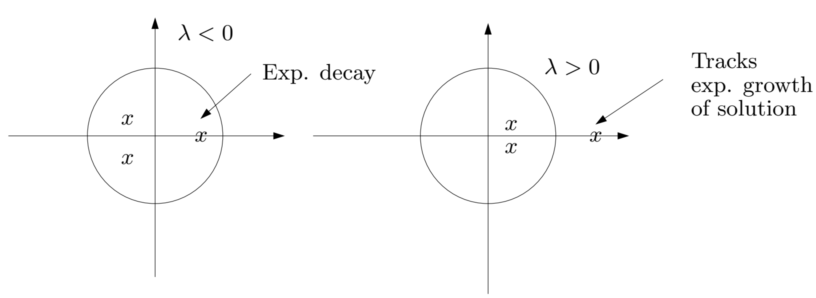
To generate the series exp for the root $G_0 = 1$ we use the recursion

$$\begin{aligned}
G &= 1 + r(1-5G+19G^2+9G^3)/G^2\\
G_0 &= 1, \quad G_1 = 1 + 24r, \ldots
\end{aligned}$$

To generate the series exp for the roots $G_0 = 0$ we use the recursion

$$\begin{aligned}
G^2 &= r(1-5G+19G^2+9G^3)/(G-1)\\
G_0 &= 0; \quad G_1 = \pm i r^{1/2}; \qquad G_2 = \pm i r^{1/2} + 3r + \ldots\\
\therefore G &= \begin{cases} 1 + 24r + O(r^2)\\ \pm i r^{1/2} + 3r + O(r^{3/2}) \end{cases}
\end{aligned}$$

are the appropriate expansions for G.



$$Y_n \sim C_1(1+24r+\ldots)^n + C_2(ir^{1/2}+3r+\ldots)^n + C^3(-ir^{1/2}+3r+\ldots)^n$$

Tracks $e^{\lambda x_n}$ Parasitic solutions – decay

BDF Methods – Good for stiff problems:

- Extension of Backward Euler
- Only evaluate $f(x,y)$ once at the end of the timestep
- Use high order backward difference approximations to y'.

Recall :

$$\begin{aligned}
y_{n+1} &= Ey_n = (1+hD+\frac{hD^2}{2!}+\ldots)y_n = e^{hD} \\
hD &= \ln E \qquad E=(1-\nabla)^{-1} \\
&= -\ln(1-\nabla) \\
&= \sum_{j=1}^{\infty}\frac{\nabla^j}{j} \\
y' &\simeq \frac{1}{h}\sum_{k=1}^{P}\frac{\nabla^k}{k}\, y_n = f(x_n,y_n) \qquad \text{A } p\text{th order method (LTE } O(h^{p+1}) \rightarrow \text{ GTE } O(h^p))
\end{aligned}$$

or $\boxed{\sum_{i=0}^{P}\alpha_i Y_{n-i} = h\beta_0 f_n}$

BDF1: $\nabla y_n = hf_n \Rightarrow \boxed{Y_n = Y_{n-1}+hf_n}$ Backward Euler $O(h)$

BDF2:

$$\frac{1}{2}\nabla^2 y_n + \nabla y_n = \frac{1}{2}(y_n - 2y_{n-1}+y_{n-2}) + (y_n - y_{n-1}) = hf_n$$

$$\frac{3}{2}y_n - 2y_{n-1} + \frac{1}{2}y_{n-2} = hf_n$$

$$\boxed{Y_n - \tfrac{4}{3}Y_{n-1} + \tfrac{1}{3}Y_{n-2} = \tfrac{2}{3}hf_n}$$

3.5 **Predictor Correct Methods**

Split ME into two steps

$$(1) \qquad y_{i+1}^{(0)} = y_i + hf(x_i, y_i) \qquad \text{predictor}$$

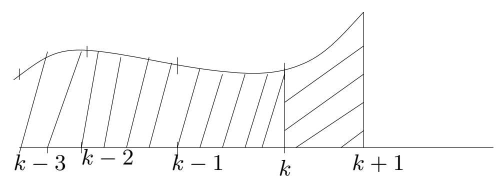
$$(2) \qquad y_{i+1}^{(k+1)} = y_i + \frac{h}{2}\left[f(x_i, y_i) + f\left(x_{i+1}, y_{i+1}^{(k)}\right)\right] \qquad k = 0, \ldots, \quad \text{corrector loop}$$

$$\text{Stop when} \qquad \frac{|y_i^{(k)} - y_i^{(k-1)}|}{|y_i^{(k)}|} < \varepsilon$$

The first step in functional iteration $x = g(x)$ $\quad |g'(x_0)| < 1$.

The Milne-Simpson Method: – More accurate is not always better.

Predictor: (Explicit)



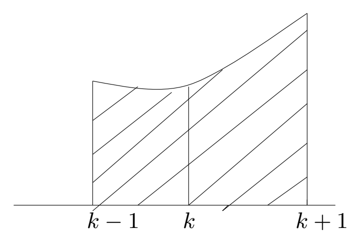
$$y_{k+1} = y_{k-3} + \int_{x_{k-3}}^{x_{k+1}} f(t, y(t))dt$$

$$||$$

$$P_3$$

$$= y_{k-3} + \frac{4h}{3}(2f_{k-2} - f_{k-1} + 2f_k) + O(h^5)$$

Corrector: (Implicit)



$$y_{k+1} = y_{k-1} + \int_{x_{k-1}}^{x_{k+1}} f(t, y(t))dt$$

$$= y_{k-1} + \frac{h}{3}(f_{k-1} + 4f_k + f_{k+1}) + O(h^5)$$

Stability of correctors: $y' = \lambda y \qquad y(0) = 1$

MILNE: $y_{n+1} = y_{n-1} + \frac{h}{3}(\lambda y_{n+1} + 4\lambda y_n + \lambda y_{n-1})$

$$\left(1 - \frac{h\lambda}{3}\right) y_{n+1} - \frac{4\lambda h}{3} y_n - \left(1 + \frac{h\lambda}{3}\right) y_{n-1} = 0$$

$$(1 - r)y_{n+1} - 4ry_n - (1 + r)y_{n-1} = 0$$

Looking for solutions of the form:

$$y = G^n$$

which gives a second order polynomial for G in terms of $h\lambda$. Although it is easy to write down the roots $\theta_{1,2}$ of this polynomial it is sufficient to study stability for small λh, which can be done using a Taylor series expansion.

Tables of Multistep methods and their stencils
Adams-Bashforth: − Explicit

Number of Steps	Order	b_s	b_{s-1}	b_{s-2}	b_{s-3}	b_{s-4}
1	1	0	1	(Euler)		
2	2	0	$\frac{3}{2}$	$-\frac{1}{2}$		
3	3	0	$\frac{23}{12}$	$-\frac{16}{12}$	$\frac{5}{12}$	
4	4	0	$\frac{55}{24}$	$-\frac{59}{24}$	$\frac{37}{24}$	$-\frac{9}{24}$

		$n+s$	$n+s-1$		n
Stencil:	a_j :	○	●		
	b_j :		●	●	●

○ = yet to be determined ● = known values.
Adams-Moulton: − Implicit

Number of Steps	Order	b_s	b_{s-1}	b_{s-2}	b_{s-3}	b_{s-4}
1	1	1			Backward Euler	
1	2	$\frac{1}{2}$	$\frac{1}{2}$		Trapezoidal Method	
2	3	$\frac{5}{12}$	$\frac{8}{12}$	$-\frac{1}{12}$		
3	4	$\frac{9}{24}$	$\frac{19}{24}$	$-\frac{5}{24}$	$\frac{1}{24}$	
4	5	$\frac{251}{720}$	$\frac{646}{720}$	$-\frac{264}{720}$	$\frac{106}{720}$	$-\frac{19}{720}$

		$n+s$	$n+s-1$		n
Stencil:	a_j :	○	●		
	b_j :	○	●	●	●

Backward Difference Formulae

Number of Steps	Order	a_s	a_{s-1}	a_{s-2}	a_{s-3}	a_{s-4}	b_s
1	1	1	-1		Backward Euler		1
2	2	1	$-\frac{4}{3}$	$\frac{1}{3}$			$\frac{2}{3}$
3	3	1	$-\frac{18}{11}$	$\frac{9}{11}$	$-\frac{2}{11}$		$\frac{6}{11}$
4	4	1	$-\frac{48}{25}$	$\frac{36}{25}$	$-\frac{16}{25}$	$\frac{3}{25}$	$\frac{12}{25}$

	$n+s$	$n+s-1$	$n+s-2$	n
Stencil: a_j :	$\circ$	$\bullet$	$\bullet$	$\bullet$
b_j :	$\circ$			

Folklore
RK vs. Adams Methods

	RK	Adams	Implicit
• Function Evaluations Expensive	Poor	Preferred	
• Function Evaluations Inexpensive & Moderate Accuracy	More Efficient	Less Efficient	
• If Storage is at a Premium	Better	Worse	
• Accuracy over a wide range of Tolerances	Not Suitable	Preferred	
• Problem Stiff -Widely varying time scales present in the problem -Stability is more of a constraint than accuracy -Explicit Methods don't work.			BDF2

A perspective on second order methods

Method	Explicit/ Implicit	Function Evaluations Per Step	Error Const	Storage	Stability
RK2	Explicit	2	1/6	$2N$	*FIGURE*
TR	Implicit	–	1/12	$2N$	A-Stable Weak Decay
AB2	Explicit	1	5/12	$3N$	*FIGURE*
2BDF	Implicit	–	1/6	$3N$	A-Stable L-Stable

Notes:

- For PDE problems storage is a big concern. Since the spatial discretization introduces errors there is no point using high order time stepping schemes so second order is usually OK.
- If the problem is very stiff 2BDF is recommended otherwise AB2 (possibly with a predictor corrector to control error).
- For simpler problems for which storage is not a problem and in which the system is not stiff, use RK4 (or RKF45 for error control) if minimizing computational time is not a priority. Or use AB4 (or APC4 with error control) otherwise.