Multistep Methods

- Idea: Use more previous timesteps to get a better approximation rather than more gradient evaluations per timestep.

- Because we are using more than one timestep we end up with higher order difference equation that we are using to model the first order ODE. $y' = f(x, y)$. We have to be careful that the additional (sometimes spurious) solutions do not end up corrupting the numerical solution.

- General Multistep Method:

$$\sum_{k=0}^{N} a_k y_{j+k} = h \sum_{k=0}^{N} b_k f_{j+k}$$

  and define the corresponding characteristic polynomials $P_N(\theta)$ and $Q_N(\theta)$ as follows: $P_N(\theta) = \sum_{k=0}^{N} a_k \theta^k$ and $Q_N(\theta) = \sum_{k=0}^{N} b_k \theta^k$

- Consistency: It can be shown (exercise) that the method is consistent if and only if $P_N(1) = 0$ and $P'_N(1) = Q_N(1)$.

- 0-stability: The method is said to be 0-stable provided the roots θ_k of $P_N(\theta) = 0$ are either such that $|\theta_k| < 1$ or $|\theta_k| = 1$ in which case the roots are simple.

Eg: **The Leapfrog Method**:

Idea: Use central differences to approximate the first derivative rather than the forward/backward difference schemes used in Euler's methods and the multistage methods.

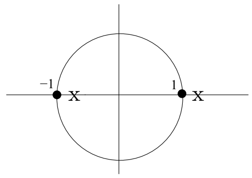
We obtain the leapfrog scheme:

$$\boxed{Y_{n+1} = Y_{n-1} + 2hf(x_n, Y_n), \qquad Y_0 = h_0.}$$

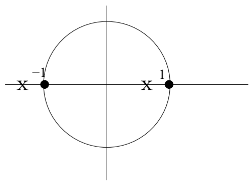
As usual, a Taylor series expansion shows that the truncation error for this method is of $O(h^2)$.

Perturbation argument for Leapfrog:

$$\begin{aligned}
y_{n+1} &= y_{n-1} + 2hf(x_n, y_n) \qquad f = \lambda y \\
y_n &= G^n \\
G^2 &- 2(\lambda h)G - 1 = 0 \qquad\qquad y_n = e^{in\alpha} \\
G^2 &= 1 + 2\varepsilon G \qquad \varepsilon = \lambda h \qquad e^{i(n+1)\alpha} - 2\lambda h e^{in\alpha} - e^{i(n-1)\alpha} \\
G &= \pm(1 + 2\varepsilon G)^{1/2} \qquad\qquad e^{i\alpha} - 2\lambda h - e^{i\alpha} = 0 \\
&= [1 + \varepsilon G - \frac{1}{2}(\varepsilon G)^2 + \ldots] \qquad \lambda h = \frac{e^{i\alpha} - e^{-i\alpha}}{2} = i \sin\alpha \\
&\sim (1 + \varepsilon G + \ldots) \\
G = G_1 + \epsilon G_2 + \ldots \Rightarrow &\quad G_1 = \pm 1, \quad G_1 + \epsilon G_2 = \pm(1 + \varepsilon G_1) = \pm 1 + \varepsilon
\end{aligned}$$



$Re\lambda > 0$ unstable



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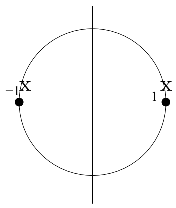


$Re\lambda = 0$

could be stable provided h
is small enough

In fact $G_1 G_2 = -1 \Rightarrow$ for stability G_1, G_2 must be on unit disk

$$
\begin{aligned}
\therefore G_1 &= e^{i\alpha} \quad G_2 = e^{-i\alpha} \\
G &= z \pm \sqrt{z^2+1} \qquad z = \lambda h \\
G^2 &- 2zG - 1 = 0 \Rightarrow \quad z = \frac{G^2-1}{2G} = \frac{1}{2}(G - G^{-1}) \\
\therefore z &= \frac{1}{2}(e^{i\alpha} - e^{-i\alpha})
\end{aligned}
$$

$$\boxed{z = i \sin\alpha}$$

Explicit Multistep Methods – Adams Bashforth

A-B2: $y_n = y_{n-1} + h\alpha f(x_{n-1}, y_{n-1}) + h\beta f(x_{n-2}, y_{n-2}) = y_{n-1} + h\alpha f_{n-1} + h\beta f_{n-2}$

Expand each of these terms in (1) about x_n, y_n in a Taylor Series.

$$
\begin{aligned}
y_n &= (y_n - hy_n' + \frac{h^2}{2} y_n'' + \ldots) + \alpha h \left\{ f_n - hf_n' + \ldots \right\} + \beta h \left\{ f_n - 2hf_n' + \ldots \right\} \\
&= y_n + h\left(-1 + \alpha + \beta\right) y_n' + h^2 y_n'' \left(\frac{1}{2} - \alpha - 2\beta \right) + O(h^3)
\end{aligned}
$$

In order for the terms up to $O(h^2)$ to vanish we require

$$\left. \begin{array}{c} -1 + \alpha + \beta = 0 \\ \frac{1}{2} - \alpha - 2\beta = 0 \end{array} \right\} \Rightarrow \beta = -\frac{1}{2}, \quad \alpha = \frac{3}{2}$$

We obtain the second order Adams-Bashforth Method AB2:

$$\boxed{Y_{n+1} = Y_n + \tfrac{3}{2} hf(x_n, Y_n) - \tfrac{1}{2} hf(x_{n-1}, Y_{n-1})}$$

- Accuracy $O(h^2)$

- Need Y_0 and Y_1 to start the time-stepping – use RK4 to find Y_1
- Stability: Consider $y' = \lambda y$

$$Y_{n+1} = \left(1 + \frac{3h\lambda}{2}\right) Y_n - \frac{h\lambda}{2} Y_{n-1} \text{ – A second order DCE}$$

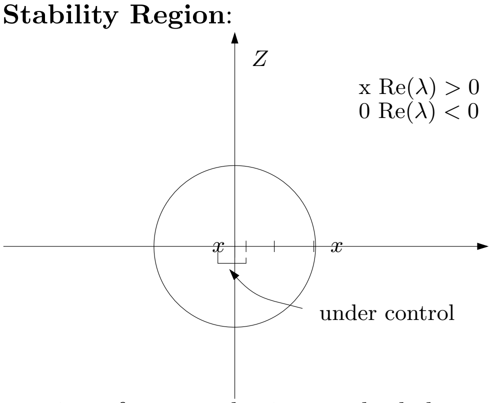
Look for solutions of the form $Y_n = G^n$

$$G^2 - (1 + 3z/2)G + \frac{z}{2} = 0$$

As $z \to 0$, $G^2 - G = 0$ the Zero Stability Polynomial which has roots

$$\begin{aligned} G_1 &= 1 \quad \text{a root shared by all consistent methods} \\ G_2 &= 0 \quad \text{which is the spurious root in this case – under control} \\ \text{For } z \text{ small} \quad G &= \left\{ \left(1 + \frac{3}{2}z\right) \pm \sqrt{(1 + 3/2z)^2 - 4z/2} \right\} /2 \\ &= \left\{ \begin{array}{l} 1 + z + O(z^2) \\ \frac{z}{2} + O(z^2) \end{array} \right. \end{aligned}$$

Stability Region:



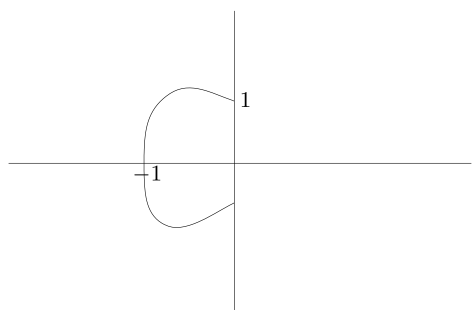


Illustration of a perturbation method that can be used to derive an expression for the roots to the characteristic equation in the limit $z \to 0$.

$$G^2 - \left(1 + \frac{3z}{2}\right) G + \frac{z}{2} = 0 \qquad (*)$$

$$z = 0 \Rightarrow \qquad G(G-1) = 0 \qquad G = 0, 1.$$

Assume that G has a power series expansion in powers of z:

$$G = G_0 + G_1 z + G_2 z^2 + \ldots$$

Plug into (*): $(G_0 + G_1 z + \ldots)^2 - \left(1 + \frac{3z}{2}\right)(G_0 + G_1 z + \ldots) + \frac{z}{2} = 0$

Expand and collect powers of z:

$$z^0 > \qquad G_0^2 - G_0 = 0 \qquad G_0 = 0, 1$$

$$z' > \qquad 2G_0 G_1 - \frac{3}{2}G_0 - G_1 + \frac{1}{2} = 0$$

$$\therefore G_1(2G_0 - 1) = -\frac{1}{2} + \frac{3}{2}G_0$$

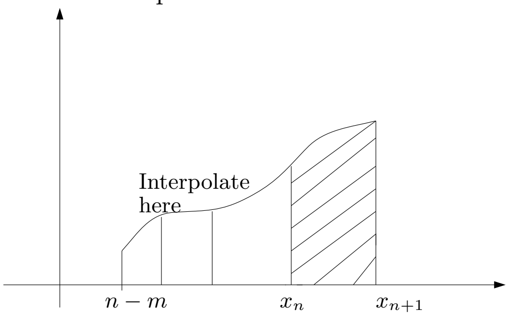
$$G_1 = \frac{-\frac{1}{2} + \frac{3}{2}G_0}{2G_0 - 1} \Rightarrow \begin{array}{l} G_0 = 0 \Rightarrow G_1 = +1/2 \\ G_0 = 1 \Rightarrow G_1 = \frac{1}{1} = 1 \end{array}$$

$$\therefore G = \left\{ \begin{array}{l} 1 + z + O(z^2) \\ 0 + \frac{z}{2} + O(z^2) \end{array} \right.$$

- This method was not needed here because we could use the quadratic formula. However, for higher order methods this technique becomes extremely useful.

- Note that the zeroth order term is the zero-stability polynomial.

To derive higher order AB methods we use the integral form of the ODE and interpolate f over previous timesteps



$$\begin{aligned}
y_{n+1} &= y_n + \int_{x_n}^{x_{n+1}} f(x, y(x))\, dx \qquad (1) \\
f_{n+s} &= E^s f_n = (1-\nabla)^{-s} = \sum_{k=0}^{m} (-1)^k \binom{-s}{k} \nabla^k f_n \\
\text{But } \Delta f_{k-1} &= \nabla f_k, \ldots, \nabla^j f_i = \Delta^j f_{i-j} \\
\therefore f_{n+s} &= \sum_{k=0}^{m} (-1)^k \binom{-s}{k} \Delta^k f_{n-k} \qquad (2) \\
\text{where } \binom{y}{k} &= \begin{cases} y(y-1)\ldots(y-k+1)/k! & k>0 \\ 1 & k=0 \end{cases}
\end{aligned}$$

Make the transformation of variables $s = (x - x_n)/h$; $dx = hds$

$$\begin{aligned}
\therefore y_{n+1} &= y_n + h \int_0^1 \sum_{k=0}^{m} (-1)^k \binom{-s}{k} \Delta^k f_{n-k}\, ds \\
&= y_n + h \{\gamma_0 f_n + \gamma_1 \Delta f_{n-1} + \ldots + \gamma_m \Delta^m f_{n-m}\} \\
\text{where } \gamma_k &= (-1)^k \int_0^1 \binom{-s}{k} ds \\
\gamma_0 &= 1 \\
\gamma_1 &= (-1) \int_0^1 \frac{(-s)}{1}\, ds = \frac{1}{2} \\
\gamma_2 &= (-1)^2 \int_0^1 \frac{(-s)(-s-1)}{2}\, ds = \frac{5}{12} \\
\gamma_3 &= \frac{3}{8} \\
\gamma_4 &= \frac{251}{720}
\end{aligned}$$