Lecture 18

Last time we did multi-step methods

$$\frac{dy}{dx} = f(x,y) \qquad y(x_0) = y_0$$

Adam-Bashforth formula of order m

~~$y_{n+1} = y_n + h \int_0^1 \{ \gamma_0 f_n$~~

$$y_{n+1} = y_n + h\{\gamma_0 f_n + \gamma_1 \nabla f_n + \cdots + \gamma_m \nabla^m f_m\}$$

$$\gamma_k = (-1)^k \int_0^1 \binom{-s}{k} ds$$

AB - order 2 formula

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

$$f_i = f(x_i, y_i)$$

AB - order 4 formula

$$y_{n+1} = y_n + \frac{h}{24}(55f_n - 59f_{n-1} + 37f_{n-2} - 9f_{n-3})$$

Predictor - corrector method

1. Euler - Trapezoidal rule

↑ Predictor ↑ corrector

$$y_{n+1}^{(0)} = y_n + h f(x_n, y_n)$$

$$y_{n+1} = y_{n+1}^{(1)} = y_n + \frac{h}{2}\left[f(x_n, y_n) + f(x_{n+1}, y_{n+1}^{(0)})\right]$$

Usually corrector is applied only once.

Adam-Moulton Method of order m

$$y_{n+1} = y_n + h\left(\gamma_0' f_{n+1} + \gamma_1' \nabla f_{n+1} + \cdots + \gamma_{m+1}' \nabla^{m+1} f_{n+1}\right)$$

$$\gamma_k' = (-1)^k \int_0^1 \binom{1-s}{k} ds$$

$m = 2$

$$y_{n+1} = y_n + \frac{h}{24}\left(9 f_{n+1} + 19 f_n - 5 f_{n-1} + f_{n-2}\right)$$

Adam-Bashforth corrector
Adam-Moulton predictor

$y' = f(x,y)$

$x_n = x_0 + nh$

$(y_0, f_0), \ldots, (y_3, f_3)$ given

$$y_{n+1}^{(0)} = y_n + \frac{h}{24}\left[55 f_n - 59 f_{n-1} + 37 f_{n-2} - 9 f_{n-3}\right]$$

$$y_{n+1} = y_{n+1}^{(1)} = y_n + \frac{h}{24}\left[9 f(x_{n+1}, y_{n+1}^{(0)}) + 19 f_n - 5 f_{n-1} + f_{n-2}\right].$$

Corrector applied only once usually

Local error control

$$y(x_{n+1}) - y_{n+1}^{(1)} \cong \frac{-19}{270}\left(y_{n+1}^{(1)} - y_{n+1}^{(0)}\right) = D_{n+1}$$

↑ we need to estimate this

↑ computable

Usually, we need $E_1 \le \left|\frac{D_{n+1}}{h}\right| \le E_2$

$\left|\frac{D_{n+1}}{h}\right| > E_2$ then half the step size

$\left|\frac{D_{n+1}}{h}\right| < E_1$ then double step size

Lecture 18

Simple difference equations

A difference equation of order N is a relation between the differences

$y_n = \Delta^0 y_n \quad \Delta^1 y_n = y_{n+1} - y_n, \quad \Delta^2 y_n, \ldots, \Delta^N y_n$

of a number sequence (i.e.,

$$(*) \quad \Delta^N y_n = f(n, y_n, \Delta y_n, \ldots, \Delta^{N-1} y_n)$$

Recall $\Delta y_n = y_{n+1} - y_n$

$\Delta^k y_n = \Delta(\Delta^{k-1} y_n)$ for $k \geq 2$.

A solution to $(*)$ is a sequence $y_m, y_{m+1}, \ldots$ ... of numbers such that $(*)$ holds for $n = m, m+1, \ldots$

If $(*)$ is a linear difference equation then $(*)$ can be written explicitly in terms of y_j's as

$$y_{n+N} + a_{n,N-1} y_{n+N-1} + \ldots + a_{n,1} y_n = b_n$$

Examples of linear difference equation

$$y_{n+1} - y_n = 1 \qquad \text{for all } n \geq 0$$

$$y_{n+1} - y_n = n \qquad \forall\, n \geq 0.$$

$$y_{n+1} - (n+1)y_n = 0 \qquad \text{for all } n \geq 0$$

$$y_{n+2} - (2\cos r)\, y_{n+1} + y_n = 0 \qquad \text{for all } n$$

By direct substitution these equations have solutions

$$y_n = n + c$$

$$y_n = \frac{n(n-1)}{2} + c$$

$$y_n = cn!$$

$$y_n = c \cos rn$$

$\forall\, n \geq 0$

with c an arbitary constant

We consider in detail a homogeneous linear difference equation with constant coefficients

$$(*) \quad y_{n+N} + a_{N-1} y_{n+N-1} + \cdots + a_0 y_n = 0$$

We seek solution of the form $y_n = \beta^n$ for all n.

Substituting in $(*)$ we get

$$\beta^{n+N} + a_{N-1} \beta^{n+N-1} + \cdots + a_0 \beta^n = 0$$

dividing by β^n we obtain <u>characteristic equation</u>

$$p(\beta) = \beta^N + a_{N-1} \beta^{N-1} + \cdots + a_n$$

The characteristic polynomial of degree N

We first assume that its zeros $\beta_1, \beta_2, \ldots, \beta_N$ are distinct. Then $\beta_1^n, \beta_2^n, \ldots, \beta_N^n$ are all solutions of $(*)$

By linearity it follows that

$$(**) \quad y_n = c_1 \beta_1^n + c_2 \beta_2^n + \cdots + c_N \beta_N^n \quad \text{for all } n$$

for arbitary constants c_i is also a solution of $(*)$.

It can be shown that $(**)$ is the general solution of $(*)$

Example

$$y_{n+3} - 2y_{n+2} - y_{n+1} + 2y_n = 0$$

char polynomial

$$\beta^3 - 2\beta^2 - \beta + 2 = 0$$

The roots of this polynomial equation is $1, -1, 2$.

So general solution is

$$y_n = c_1 (1)^n + c_2 (-1)^n + c_3 2^n$$
$$= c_1 + c_2 (-1)^n + 2^n c_3$$

If the first N-1 values of y_n are given then we can solve (*) explicitly for all succeeding values of n

Example $y_{n+3} - 2y_{n+2} - y_{n+1} + 2y_n = 0$

$y_0 = 0, \quad y_1 = 1, \quad y_2 = 1$

Then $y_3 = 2(1) + 1 - 0 = 3$

$y_4 = 5, \quad y_5 = 11$ etc.

This does not give closed formula for y_n

Gen soln is

$$y_n = c_1 + (-1)^n c_2 + 2^n c_3$$

Using initial value $y_0 = 0, \; y_1 = 1, \; y_2 = 1$

we get

$$0 = c_1 + c_2 + c_3$$
$$1 = c_1 - c_2 + 2c_3$$
$$1 = c_1 + c_2 + 4c_3$$

Soln is $c_1 = 0, \; c_2 = -\frac{1}{3}, \; c_3 = \frac{1}{3}$.

So the closed form of sol^n of initial value problem is

$$y_n = -\frac{1}{3}(-1)^n + \frac{2^n}{3}.$$

If the characteristic polynomial has pairs of conjugate-complex zeros the solution can still be expressed in real form.

Thus if ~~$\alpha - i\beta$~~ $\beta_1 = \alpha + i\beta$, $\beta_2 = \alpha - i\beta$

we express β_1, β_2 in polar form

$$\beta_1 = r e^{i\theta} \qquad \beta_2 = r e^{-i\theta}$$

where $r = \sqrt{\alpha^2 + \beta^2}$ $\qquad \theta = \tan^{-1}(\beta/\alpha)$

Then the solution of (*) corresponding to this pair of zeros is

$$c_1 \beta_1^n + c_2 \beta_2^n = c_1 r^n e^{in\theta} + c_2 r^n e^{-in\theta}$$

$$= r^n \left(c_1 (\cos n\theta + i \sin(n\theta)) + c_2 (\cos n\theta - i \sin(n\theta)) \right)$$

$$= r^n c_1' \cos n\theta + r^n c_2' \sin n\theta$$

where $c_1' = c_1 + c_2$ $\qquad c_2' = i(c_1 - c_2)$

Example

$$y_{n+2} - 2y_{n+1} + 2y_n = 0$$

char polynomial $\beta^2 - 2\beta + 2 = 0$

$\beta_1 = 1+i$ $\beta_2 = 1-i$ root

$r = \sqrt{2}$ $\theta = \pi/4$

So gen solution

$$y_n = (\sqrt{2})^n \left(C_1 \cos \frac{n\pi}{4} + C_2 \sin \frac{n\pi}{4} \right)$$

We are solving

$$(*) \quad y_{n+N} + a_{N-1} y_{n+N-1} + \cdots + a_0 y_n = 0$$

char polynomial

$$P(\beta) = \beta^N + a_{N-1}\beta^{N-1} + \cdots + a_0 = 0$$

Suppose β_1 is a double root of $P(\beta)$

Then second solution of (*) is $n\beta_1^n$

To verify this note that if β_1 is a double root of $P(\beta)$ then $P(\beta_1)=0$ and $P'(\beta_1)=0$

Substituting $y_n = n\beta_1^n$ in (*) we get-

$$(n+N)\beta_1^{n+N} + a_{N-1}(n+N-1)\beta_1^{n+N-1} + \cdots + a_0 n\beta_1^n$$

$$= \beta_1^n \left\{ \begin{array}{l} n(\beta_1^N + a_{N-1}\beta_1^{N-1} + \cdots + a_0) \\ + \beta_1(N\beta_1^{N-1} + a_{N-1}(N-1)\beta_1^{N-2} + \cdots + a_1) \end{array} \right\}$$

$$= \beta_1^n (n P(\beta_1) + \beta_1 P'(\beta_1))$$

$$= 0.$$

It can also be shown that the two solutions β_1^n and $n\beta_1^n$ are linearly independent.

Example

$$y_{n+3} - 5y_{n+2} + 8y_{n+1} - 4y_n = 0$$

Char polynomial

$$\beta^3 - 5\beta^2 + 8\beta - 4 = 0$$

roots are 2, 2, 1

Gen soln

$$y_n = c_1 2^n + c_2 n 2^n + c_3 1^n$$

$$= 2^n (c_1 + n c_2) + c_3$$

Non-homogeneous linear diff equations with constant coefficients.

The general solution of the eqn

$$(**) \quad y_{n+N} + a_{N-1} y_{n+N-1} + \cdots + a_0 y_n = b_n$$

can be written as

$$y_n = y_n^G + y_n^P$$

where

where y_n^G is the general solution of the homogeneous system

$$y_{n+N} + a_{N-1} y_{n+N-1} + \cdots + a_0 y_n = 0$$

and y_n^P is a particular solution of (**)

Special case $b_n = b$ is a constant.

A particular solution of (**) can be obtained by setting $y_n^P = \alpha$ (a constant)

Substituting in (**) we get

$$\alpha = \frac{b}{1 + a_{N-1} + \cdots + a_0}$$

(provided denominator $\neq 0$)

Example $y_{n+2} - 2y_{n+1} + 2y_n = 1$

$y_p = \alpha$ gets $\alpha = \frac{1}{1-2+2} = 1$

so $y_p = 1$

General soln is

$$y_n = (\sqrt{2})^n \left(c_1 \cos \frac{\pi}{4} n + c_2 \sin \frac{\pi}{4} n \right) + 1$$

Stability of Numerical methods

It was observed that some methods give errors in solution much larger than would be expected from the discretization error alone. However as the step size h was made smaller these errors for a fixed value of x became larger rather than smaller

Consider Milne's method

$$y_{n+1} = y_{n-1} + 2hf_n$$

for which the local discretization error is

$$\frac{1}{6} h^3 y'''(\xi).$$

We would expect this method to give more accurate result for h fixed than Euler method whose local error is $O(h^2)$

Consider however the following simple problem

$$y' = -2y + 1 \qquad y(0) = 1$$

whose exact sol^n is $y = \frac{1}{2}e^{-2x} + \frac{1}{2}$.

Taking $h = 1/32$

we get $y(4.0) = 0.5001292$ by Euler method

$$\text{error} = -0.0000386$$

while $y(4.0) = 0.5284545$ by Milne's method

$$\text{error} = 0.0282768$$

Beyond $x = 4$ Milne's method has no significant digits of accuracy.

We look at the eqn more carefully

$$f_n = -2y_n + 1$$

$$y_{n+1} = y_{n-1} + 2hf_n$$

$$y_{n+1} = y_{n-1} - 4hy_n + 2h$$

So we get the difference equation

$$y_{n+1} + 4hy_n - y_{n-1} = 2h$$

$$y_n^p = \alpha$$

$$\alpha = \frac{2h}{1+4h-1} = \frac{1}{2}$$

$$y_n = c_1 \beta_1^n + c_2 \beta_2^n + \frac{1}{2}$$ is general solution

where β_1, β_2 are roots of the characteristic eqn $\beta^2 + 4h\beta - 1 = 0$

roots

$$\beta_1 = -2h + \sqrt{1+4h^2}, \quad \beta_2 = -2h - \sqrt{1+4h^2}$$

~~So β_1~~ we expand $\sqrt{1+4h^2}$ in Taylor series

$$\beta_1 = 1 - 2h + O(h^2)$$

$$\beta_2 = -(1+2h) + O(h^2)$$

$$y_n = c_1 \left(1 - 2h + O(h^2)\right)^n + c_2 (-1)^n \left(1 + 2h + O(h^2)\right)^n + 1/2$$

now $\lim_{t \to 0} (1+t)^{1/t} = e$

$n = \frac{x_n}{h}$. it follows that for fixed

x_n

$$\lim_{h\to 0}(1+2h)^n = \lim_{h\to 0}(1+2h)^{\frac{1}{2h}\cdot 2x_n}$$

$$= e^{2x_n}$$

Similarly $\lim_{h\to 0}(1-2h)^n = e^{-2x_n}$

Hence as $h\to 0$ the solution approach

$$y_n = \underbrace{c_1 e^{-2x_n} + \frac{1}{2}}_{\text{true sol}^n} + \underbrace{c_2(-1)^n e^{2x_n}}_{\text{extraneous}}$$

The second term is extraneous and arises only because we have replaced a first order differential equation by a second order difference equation.

Imposing the initial condition will if all arithmetic operations are exact, result in choosing $c_2 = 0$.

In practise however some errors will be introduced primarily due to round-off or to inexact starting values and hence C_2 will not be zero.

A small error will therefore be introduced at each step of the integration and this error will subsequently be magnified because it is multiplied by the exponentially increasing factor $(-1)^n e^{2x_n}$.

This leads to completely incorrect results.

Loosely speaking we can say that a method is unstable if errors introduced into the calculations grow at an exponential rate as the computation proceeds.

One-step methods like those of R-K type do not exhibit any Numerical instability for h suff small. [They have other types of instability which we have not discussed]

Multistep method may in some cases be unstable for all values of h and in other cases for a range of values of h.

To determine whether a given multistep method is stable we can proceed as follows.

If the multistep method leads to a difference equation of order k, find the roots of the characteristic equation corresponding to homogeneous difference equation.

Call these β_i $(i=1,2,\ldots,k)$. The general solution of the homogeneous diff equation is

$$y_n = c_1 \beta_1^n + c_2 \beta_2^n + \ldots + c_k \beta_k^n$$

One of these solution, say β_1^n will tend to the exact solution of the differential equation as $h \to 0$.

All the other solution are extraneous. A multistep method is defined to be strongly stable if the extraneous roots satisfy as $h \to 0$ the condition

$$|\beta_i| < 1 \quad \text{for } i = 2, 3, \ldots k.$$

Under this condition any error introduced into the computation will decay as n - increase

Note that if any of the extraneous β_i are greater than one in magnitude the errors will grow exponentially.

For the general differential equation $y' = f(x,y)$ it would be impossible to obtain the roots of β_i of the characteristic eqn. A consideration of the special equation $y' = \lambda y$ λ constant is usually considered sufficient however to give an indication of the stability of a method.

We consider first Adam-Bashforth fourth order method.

For $y' = \lambda y$ we obtain a recursion

$$y_{n+1} - y_n - \frac{h\lambda}{24}(55y_n - 59y_{n-1} + 37y_{n-2} - 9y_{n-3}) = 0$$

The char equation for this diff eqn is

$$\beta^4 - \beta^3 - \frac{h\lambda}{24}(55\beta^3 - 59\beta^2 + 37\beta - 9) = 0$$

The roots of this eqn are of course functions of $h\lambda$.

We write the equation as

$$(*) \quad \rho(\beta) + h\lambda\sigma(\beta) = 0$$

where $\rho(\beta) = \beta^4 - \beta^3$

$$\sigma(\beta) = \frac{-1}{24}(55\beta^3 - 59\beta^2 + 37\beta - 9)$$

As $h \to 0$ $(*)$ reduces to $\rho(\beta) = 0$

whose roots are $\beta_1 = 1$, $\beta_2 = \beta_3 = \beta_4 = 0$

For $h \neq 0$ the general solution will be of the form

$$y_n = c_1\beta_1^n + c_2\beta_2^n + c_3\beta_3^n + c_4\beta_4^n$$

It can be shown that β_1^n approaches the desired solution of $y' = \lambda y$ as $h \to 0$ while the other roots correspond to extraneous solutions

The roots of $(*)$ are continuous function of h

So for h small enough

$$|\beta_i| < 1 \quad \text{for } i = 2, 3, 4$$

So the Adam-Bashforth method is strongly stable

All multistep method lead to char eqn in the form (*) whose left hand side is called the stability polynomial. A method is strongly stable if all root of $P(\beta) = 0$ have magnitude less than one except for the simple root β_1.

Next we investigate the stability properties of Milnes method given by

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

again setting $y' = \lambda y$ we obtain

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

So its char eqn becomes

(**) $\rho(\beta) + h\lambda\sigma(\beta) = 0$

with $\rho(\beta) = \beta^2 - 1$

$\sigma(\beta) = \beta^2 + 4\beta + 1$

This time $\rho(\beta) = 0$ has roots $\beta_1 = 1$, $\beta_2 = -1$

So Milne's method is not strongly stable.

To see implication of this we compute the roots of the stability polynomial (**).

For h small

$$\beta_1 = 1 + \lambda h + \mathcal{O}(h^2)$$

$$\beta_2 = -\left(1 - \frac{2h}{3}\right) + \mathcal{O}(h^2)$$

So general sol^n is

$$y_n = c_1\left(1 + \lambda h + \mathcal{O}(h^2)\right)^n + c_2(-1)^n\left(1 - \frac{\lambda h}{3} + \mathcal{O}(h^2)\right)^n$$

Set $x = \frac{x_n}{h}$ and let $h \to 0$ this sol^n approaches

$$y_n = \underbrace{c_1 e^{\lambda x_n}}_{\text{true sol}^n} + \underbrace{c_2 (-1)^n e^{-\frac{\lambda x_n}{3}}}_{\text{extraneous sol}^n}$$

In this case stability depends on the sign of λ.

If $\lambda > 0$, the desired sol^n is exponentially increasing, it is clear that the extraneous sol^n will be exponentially decreasing. So that Milnes method will be stable.

On the other hand if $\lambda < 0$ then Milne's method will be unstable as the extraneous sol^n will be exponentially increasing and will eventually swamp the desired solution.

Methods of this type whose stability depends upon the sign of λ for the test equation $y' = \lambda y$ are said to be <u>weakly stable</u>