Lecture 17

Last time we did RK-methods of ~~order 2~~ to solve initial value problems

RK-method of order 2

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

$$y(x_0) = y_0$$

$$x_i = x_0 + ih$$

$$y_{n+1} = y_n + \frac{1}{2}(k_1 + k_2)$$

$$k_1 = h f(x_n, y_n)$$

$$k_2 = h f(x_n + h, y_n + k_1)$$

RK-method of order 4

$$y_{n+1} = y_n + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4)$$

$$k_1 = h f(x_n, y_n) \qquad k_2 = h f(x_n + \tfrac{h}{2}, y_n + \tfrac{1}{2}k_1)$$

$$k_3 = h f(x_n + \tfrac{h}{2}, y_n + \tfrac{1}{2}k_2) \qquad k_4 = h f(x_n + h, y_n + k_3)$$

We also estimated error for Euler's method and we proved that Eulers method does not blow-up.

We also did Newtons forward difference formula and Newton's backward difference formula.

Newton's forward diff formula

$$x = x_0 + sh$$

$$P_n(x) = \sum_{i=0}^{n} \binom{s}{i} \Delta^i f(x_0)$$

Newton's backward-difference formula

Lecture 17

Multi-step formulas

Euler's method, Taylors algorithm of order k and RK-methods are one step method. They require information about the solution at a single point $x = x_n$ from which the methods proceed to obtain y at the next point $x = x_{n+1}$.

Multistep methods make use of information about the solution at more than one point.

Let us assume that we already obtained approximation to y at a number of equally spaced points say $x_0, x_1, \ldots, x_n$.

One class of multi-step method is based on the principle of numerical integration.

If we integrate the differential equation $y' = f(x,y)$ from x_n to x_{n+1} we will have

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

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

To carry out the integration we approximate $f(x,y(x))$ by a polynomial which interpolates $f(x,y(x))$ at $m+1$ pts $x_n, x_{n-1}, \ldots, x_{n-m}$

This is conveniently done by the so-called Newton backward difference formula

$$P_n(x) = \sum_{k=0}^{m} (-1)^k \binom{-s}{k} \nabla^k f_n$$

$$x = x_n + sh$$

Put this in $(*)$ and note that

$$dx = h \, ds.$$

also $x_n \le x \le x_{n+1} \implies 0 \le s \le 1$

So we get-

$$y_{n+1} = y_n + h \int_0^1 \sum_{k=0}^{m} (-1)^k \binom{-s}{k} \nabla^k f_n \, ds \Big\{$$

$$= y_n + h \Big\{ \gamma_0 f_n + \gamma_1 \nabla f_n + \gamma_2 \nabla^2 f_n + \cdots + \gamma_m \nabla^m f_n \Big\}$$

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

Recall

$$\binom{-s}{k} = \frac{-s(-s-1)\cdots(-s-k+1)}{k!}$$

$$= (-1)^k \frac{s(s+1)\cdots(s+k-1)}{k!}$$

$$\gamma_0 = (-1)^0 \int_0^1 1 \, ds = 1$$

$$\gamma_1 = (-1)^1 \int_0^1 (-1)\, s \, ds$$

$$= \int_0^1 s \, ds = \frac{1}{2}.$$

$$\gamma_2 = (-1)^2 \int_0^1 (-1)^2 \frac{s(s+1)}{2}\, ds$$

$$= \int_0^1 \left(\frac{s^2}{2} + \frac{s}{2}\right) ds$$

$$= \frac{1}{6} + \frac{1}{4} = \frac{5}{12}$$

One can show

$$\gamma_3 = (-1)^3 \int_0^1 \binom{-s}{3} ds = \frac{3}{8}$$

$$\gamma_4 = (-1)^4 \int_0^1 \binom{-s}{4} ds = \frac{251}{720}$$

Adam-Bashforth order 2 formula

$$y_{n+1} = y_n + h\{\gamma_0 f_n + \gamma_1 \nabla f_n\}$$

$$= y_n + h\left\{f_n + \frac{1}{2}\{f(x_n, y_n) - f(x_{n-1}, y_{n-1})\}\right\}$$

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

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

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

This formula is called Adam-Bashforth method of order m.

$m = 3$ is commonly used

$$y_{n+1} = y_n + h\left(f_n + \frac{1}{2}\nabla f_n + \frac{5}{12}\nabla^2 f_n + \frac{3}{8}\nabla^3 f_n\right)$$

$$\nabla f_n = f_n - f_{n-1}$$

$$\nabla^2 f_n = f_n - 2f_{n-1} + f_{n-2}$$

$$\nabla^3 f_n = f_n - 3f_{n-1} + 3f_{n-2} - f_{n-3}$$

Substituting these we obtain

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

Derivation of local error

Error of Newton's backward formula with $m = 3$ and $k = 0$ is

$$h^4 f^{(4)}(\eta_s) \binom{-s}{4}$$

Therefore the error in x is

$$E = h \int_0^1 h^4 f^{(4)}(\eta_s) \binom{-s}{4} ds$$

$$= h^5 \int_0^1 f^{(4)}(\eta_s) \binom{-s}{4} ds$$

Since $\binom{-s}{4}$ does not change sign in $[0, 1]$ there exist a pt ξ between x_{n-3} and x_{n+1} such that

$$E = h^5 f^{(4)}(\xi) \int_0^1 \binom{-s}{4} ds$$

$$= h^{(5)} y^{(5)}(\xi) \frac{251}{720}.$$

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Algorithm for Adam-Bashforth method of orda 4

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

$$y(x_0) = y_0$$

Stepsize $h = \frac{b-a}{N}$

$$x_i = a + ih \qquad i = 0, 1, \dots, N.$$

· Determine y_1, y_2, y_3 by some other method (preferably RK-method of orda 4)

for $n \ge 3$

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

here $f_i = f(x_i, y_i)$

This method has local error of $O(h^5)$

Advantages - Disadvantages of Adam-Bashforth method

dis-advantage

It is not self-starting. We must have four successive values of $f(x,y)$ at equally spaced points before this formula can be used. Usually RK-method of order 4 is used to obtain the 4 initial values.

Advantages

1. AB method requires only one function evaluation per step compared with four evaluation per step with RK-method and are therefore considerably faster and require less computational work.
2. There is a way to control step-size h using A-B method which controls the error.

Other formulas of multistep type

Instead of integrating $f(x,y)$

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

from x_n to x_{n+1} we could for example integrate it from x_{n-p} to x_{n+1} for some integer $p \geq 0$.

So we obtain

$$\int_{x_{n-p}}^{x_{n+1}} \frac{dy}{dx} = \int_{x_{n-p}}^{x_{n+1}} f(x, y(x))$$

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

If we again interpolate at the $m+1$ pts $x_n, x_{n-1}, \cdots, x_{n-m}$ with Newton's backward formula we obtain

$$y_{n+1} = y_{n-p} + h \int_{-p}^{1} \sum_{k=0}^{m} (-1)^k \binom{-s}{k} \nabla^k f_n \, ds$$

The case $p=0$ yields A-B formulae

Some especially interesting formulae of this type corresponding to $m=1$, $p=1$ and to $m=3$, $p=3$

The formulae are

$$y_{n+1} = y_{n-1} + 2h f_n$$

Local error $E = \frac{h^3}{3} y^{(3)}(\xi)$

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

Local error $E = \frac{14}{45} h^5 y^{(5)}(\xi)$

These formulae "book" better since they are of higher order.

However these formulae are subject to greater instability. (This we will study later)

Predictor - Corrector methods.

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

$$a = x_0 \le x \le b$$

$$y(x_0) = y_0$$

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

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

Suppose we approximate the integral above by the trapezoidal rule. This leads to the formula

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

$$n = 0, 1, 2, \ldots$$

Error in this formula is $-\left(\frac{h^3}{12}\right) y'''$ and is thus an improvement over Euler method

However (*) is an implicit equation for y_{n+1} since y_{n+1} appears as an argument on the right hand side.

If $f(x,y)$ is a non-linear equation we will not be able to solve (*) for y_{n+1} exactly.

We can however attempt to obtain y_{n+1} by means of iteration. Thus keeping x_n fixed we obtain a first approximation $y_{n+1}^{(0)}$ to y_{n+1} by means of the Euler formula

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

We then evaluate $f(x_{n+1}, y_{n+1}^{(0)})$ and substitute in the RHS of (*) to obtain

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

Next we evaluate $f(x_{n+1}, y_{n+1}^{(1)})$ and again use (*) to obtain a next approximation.

In general, the iteration is defined by

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

$k = 1, 2, \ldots$

The iteration is terminated if two successive iterates agree to the desired accuracy

Thus we use Euler's method to "predict" y_{n+1} and then use (*) to "correct".

Algorithm :- A second order predictor-corrector method.

For the differential eqn $\frac{dy}{dx} = f(x,y)$, $y(x_0) = y_0$ with h given and $x_n = x_0 + nh$ for $n = 0, 1, 2, \ldots$

1) compute $y_{n+1}^{(0)}$ from the formula

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

(2) compute $y_{n+1}^{(k)}$ $(k=1,2,\dots)$ until satisfied by

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

Example

$$\frac{dy}{dx} = x - \frac{1}{y}$$

$x \in [0, 0.2]$

$y(0) = 1$

$x_1 = 0.1, \quad x_2 = 0.2, \quad h = 0.1$

1) $y_1^{(0)} = 0.9$ by Euler's method

$y_1^{(1)} = 0.8994$

$y_1^{(2)} = 0.8994$ } by (*)

Since $y_1^{(1)}$ and $y_2^{(1)}$ agree to four places

we accept $y_1 = 0.8944$

2) By Euler method

$y_2^{(0)} = 0.7992$

By (*) we get

$$y_2^{(1)} = 0.7962$$

$$y_2^{(2)} = 0.7960$$

$$y_2^{(3)} = 0.7960$$

we accept $y_2 = 0.7960$

Question Under what conditions does the iteration defined by (*) converge?

Theorem If $f(x,y)$ and $\frac{\partial f}{\partial y}$ are continuous in x and y on the interval $[a,b]$, the inner iteration defined by (*) will converge provided h is small enough so that for $x = x_n$ and all y with $|y - y_{n+1}| \leq |y_{n+1}^{(0)} - y_{n+1}|$

$$\left|\frac{\partial f}{\partial y}\right| h < 2.$$

Proof The iteration (*) is

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

$k = 1, 2, \ldots$

Note that x_n is fixed in (*)

Set $Y^{(k)} = y_{n+1}^{(k)}$

So $Y^{(k)} = F(Y^{(k-1)})$

where $F(Y) = \frac{h}{2} f(x_{n+1}, Y) + C$

and where $C = y_n + \frac{h}{2} f(x_n, y_n)$ depends on n but not on Y.

This can be viewed as an instance of fixed pt convergence. We proved that such an iteration converges provided that $F(Y)$ is cts and satisfies

$$|F'(Y)| < 1$$

for all y with $|y - y_{n+1}| \le |y^{(0)} - y_{n+1}|$

where y_{n+1} is the fixed pt of $F(y)$

$$F'(y) = \frac{h}{2} \frac{\partial f}{\partial y}.$$

Thus iteration will converge if

$$|F'(y)| = \left|\frac{h}{2} \frac{\partial f}{\partial y}\right| < 1$$

$$\text{i.e. } h \left|\frac{\partial f}{\partial y}\right| < 2.$$

Adam - Moulton Method

This is used as a corrector for A-B method

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

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

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

We use polynomial which interpolates $f(x, y(x))$ at the points $x_{n+1}, x_n, \ldots, x_{n-m}$ for an integer $m > 0$

The Newton backward difference formula which interpolates at these $m+2$ pts

in terms of $s = \frac{x - x_n}{h}$ is

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

$$s = \frac{x - x_n}{h} \qquad \text{so} \quad ds = \frac{dx}{h}$$

$$y_{n+1} = y_n + h \int_0^1 \left(\sum_{k=0}^{m+1} (-1)^k \binom{1-s}{k} \nabla^k f_{n+1} \right) ds$$

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

$$\gamma_k' = (-1)^k \int_0^1 \binom{1-s}{k} ds \qquad k = 0, 1, \cdots, m+1$$

The first few values of γ_k' are

$\gamma_0' = 1$, $\gamma_1' = -\frac{1}{2}$, $\gamma_2' = -\frac{1}{12}$, $\gamma_3' = -\frac{1}{24}$

$\gamma_4' = -\frac{19}{720}$ (in your first textbook $\gamma_4' = -\frac{10}{720}$ is WRONG)

$$\text{Error } E = \gamma'_{m+2}\, h^{m+3}\, y^{(m+3)}(\xi)$$

The case $m=2$ is frequently used

(Adam-Moulton formula)

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

$$E = \frac{-19}{720} h^5 y^{(5)}(\xi)$$

This is a corrector formula of closed type since $f_{n+1} = f(x_{n+1}, y_{n+1})$ involves the unknown quantity y_{n+1}

Predictor used is Adam-Bashforth fourth order formula

Algorithim (The Adam-Bashforth Adam-Moulton predictor-corrector method

For the diff equation $y' = f(x,y)$ with h fixed and $x_n = x_0 + nh$ and with $(y_0, f_0), (y_1, f_1), (y_2, f_2), (y_3, f_3)$ given for each fixed $n = 3, 4, \ldots$

1. Compute $y_{n+1}^{(0)}$ using the formula

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

here $f_i = f(x_i, y_i)$

2. Compute until satisfied

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

3) If satisfied with $y_{n+1}^{(k)}$ then

set $y_{n+1} = y_{n+1}^{(k)}$

Exercise :- Show that the iteration (*) converges if $\frac{9h}{24}\left|\frac{\partial f}{\partial y}\right| < 1$

Step-Size control

Besides yielding improved accuracy the corrector formula serves another useful function. It provides an estimate of the local error which can be used to decide whether the step h is adequate for the required accuracy.

Local error of A-B method $E_{AB} = \frac{251}{720} h^5 y^{(5)}(\xi_1)$

Local error of A-M method $E_{AM} = \frac{-19}{720} h^5 y^{(5)}(\xi_2)$

Let $y_{n+1}^{(0)}$ represent value of y_{n+1} obtained by A-B method.

Let $y_{n+1}^{(1)}$ be the result obtained by AM method.

Thus (**)
$$\begin{cases} y(x_{n+1}) - y_{n+1}^{(0)} = \frac{251}{720} h^5 y^{(5)}(\xi_1) \\ y(x_{n+1}) - y_{n+1}^{(1)} = \frac{-19}{720} h^5 y^{(5)}(\xi_2) \end{cases}$$

In general $\xi_1 \neq \xi_2$. But we can assume that for x_{n+1} close to x_n $\xi_1 \approx \xi_2$.

By (**) we obtain $h^5 y^{(5)}(\xi) = \frac{720}{270} (y_{n+1}^{(1)} - y_{n+1}^{(0)})$

Substituting this in second equation above we get

$$y(x_{n+1}) - y_{n+1}^{(1)} = \frac{-19}{270} (y_{n+1}^{(1)} - y_{n+1}^{(0)})$$
$$\approx -\frac{1}{14} (y_{n+1}^{(1)} - y_{n+1}^{(0)}) = D_{n+1}$$

Thus the error of the corrected value is approximately $-\frac{1}{14}$ of the difference between the corrected and predicted values

It is advisable to use corrector only once. If accuracy of D_{n+1} is not sufficient it is better to reduce the step size than to correct more than once.

The error estimate is used in the following manner

Let us assume that we wish to keep the local error per unit step bounded as

$$E_1 \leq \frac{|D_{n+1}|}{h} \leq E_2$$

We proceed as follows

1) Use A-B formula to compute $y_{n+1}^{(0)}$

2) Use A-M formula to compute $y_{n+1}^{(1)}$

3) Compute $D_{n+1} = \frac{-1}{14}\left(y_{n+1}^{(1)} - y_{n+1}^{(0)}\right)$

4) If $E_1 \leq \frac{|D_{n+1}|}{h} \leq E_2$ then proceed to the next integration step, using the same value of h.

5) If $\frac{|D_{n+1}|}{h} > E_2$ then the step-size h is too large and should be reduced to $h/2$.

(6) If $\frac{|D_{n+1}|}{h} < E_1$, more accuracy is being obtained than necessary. Hence we can save computer time by replacing h by $2h$.