Lecture 26

Last time we did Runge-Kutta methods (in short RK-method) to solve initial value problems.

RK-method of order 2

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

$$y(x_0) = y_0 \qquad a = x_0 \le x \le b$$

$$x_i = x_0 + ih \qquad h \text{ step size}$$

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

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

RK-method of order 4

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

$$k_1 = h f(x_n, y_n) \qquad k_3 = h f\left(x_n + \frac{h}{2}, y_n + \frac{1}{2}k_2\right)$$
$$k_2 = h f\left(x_n + \frac{h}{2}, y_n + \frac{1}{2}k_1\right) \qquad k_4 = h f(x_n + h, y_n + k_3)$$

We also did Newton's forward diff formula and Newton's backward diff 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 diff formula

$$x = x_n + sh$$

$$P_n(x) = \sum_{i=0}^{n} (-1)^i \binom{-s}{i} \nabla^i f(x_n)$$

Multi-Step formulas

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

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 multistep methods 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

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

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

To carry out the integration we now approximate $f(x, y(x))$ by a polynomial which interpolates $f(x, y(x))$ at the $m+1$ pts $x_n, x_{n-1}, x_{n-2}, \ldots x_{n-m}$

This is conveniently done by the socalled Newton's backward diff formula

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

$$x = x_n + sh$$

Put this in $(*)$ and note that

$$dx = h \, ds$$

So we get

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

$$= y_n + h \left\{ \gamma_0 f_n + \gamma_1 \nabla f_n + \cdots + \gamma_m \nabla^m f_m \right\}$$

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

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

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

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

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

This formula is called Adam-Bashforth method

$m=3$ 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

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

<u>derivation of local error</u>

error of Newton's backward formula with $n=3$ and $k=0$ is

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

Therefore the error in (*) is

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

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

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

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

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

Algorithim for Adam-Bashforth method

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

$$y(x_0) = y_0$$

- step size $h = \frac{b-a}{N}$

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

- determine y_1, y_2, y_3 by some other method (preferably RK-method of order 4)

- for $n \geq 3$

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

here $f_i = f(x_i, y_i)$

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

Advantages - Disadvantages of Adam-Bashforth method

disadvantage

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

advantage

AB method require 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.

Other formulas of multistep type

Instead of integrating $f(x,y)$ in

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

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

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

If we again interpolate at the $m+1$ pts $x_n, x_{n-1}, \ldots, x_{n-m}$ 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 Adam-Bashforth formula

Some especially interesting formulas of this type are those corresponding to $m=1, p=1$ and to $m=3, p=3$.

These formulas are

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

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

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

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

These formulas "look" better since they are of higher order.

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

Predictor-Corrector methods

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

$$y(x_0) = y_0$$

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

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

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

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

Error in this formula is

$$-\left(\frac{h^3}{12}\right) y'''$$ and is thus an improvement over Euler's 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 function 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 Euler's 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".

<u>Algorithm</u> :- A second order predictor-corrector method.

For the diff equation $\frac{dy}{dx} = f(x,y)$, $y(x_0) = y_0$

with h given and $x_n = x_0 + nh$ for $n = 0, 1, 2, \ldots$

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

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

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

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

$y(0) = 1$ $\qquad x \in [0, 0.2]$

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

1) $y_1^{(0)} = 0.9$ $\qquad$ By Euler' method

$y_1^{(1)} = 0.8994$

$y_1^{(2)} = 0.8944$ $\qquad$ } by (*)

Since $y_1^{(1)}$ and $y_1^{(2)}$ agree to four places

we accept $y_1 = 0.8944$

2) By Euler's method

$y_2^{(0)} = 0.7982$

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 chosen 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

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

$k = 1, 2, \ldots$

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 iteration. We proved that such an iteration converges provided that $F'(Y)$ is continuous and satisfies

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

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

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

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

The iteration will converge if

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

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