UNIVERSITY OF AGRICULTURE, ABEOKUTA
COLLEGE OF NATURAL SCIENCES
DEPARTMENT OF COMPUTER SCIENCE

NUMERICAL ANALYSIS II
CSC 351- 3 UNITS

A MATERIAL DEVELOPED

BY

DR. O. R. VINCENT

COURSE CODE: CSC 351

COURSE TITLE: NUMERICAL ANALYSIS

NUMBER OF UNITS: 3 UNITS

COURSE DURATION: THREE HOURS PER WEEK

COURSE DETAILS:

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Office Location   Room B201, COLNAS

Other Lecturers   xxxxx

COURSE CONTENT:

Newton's central difference formular and Backward differences – stirling's formular. Numerical differentiation and integrations. Solution to ordinary differential equations. Direct and iterative methods for solution of linear system. Least square polynomial approximations. Introduction of numerical solution of partial differential equations.

COURSE REQUIREMENTS:

This is a compulsory course for all students in Computer Science and elective for stdent in Mathematics Depertment. The students will be expected to prepare charts, algorithms and write programmes in FORTRAN language are expected to be able to write a good proposal at the end of the course and present a seminar to defend their proposal.

READING LIST:

2.0

SOLUTIONS OF DIFFERENTIAL EQUATIONS

To consider:

(1)   Euler method

(2)   Improved Euler-Cauchy method (predictor – corrector method)

(3)   Runge-Kutta method

INITIAL VALUE PROBLEM

Generally, f(x, y, y') = 0, y(0) = y_0, the solution must satisfy certain initial conditions. It can be put as

$$y' = f(x, y), y(0) = y_0 \dots\dots\dots\dots\dots\dots\dots\dots\dots\dots.. (1)$$

Numerical Method for 1st Order Differential Equations

1.   Euler Method

$$y(x + h) = y(x) + hy'(x) + h^2 y''(x) + \cdots \qquad (2)$$

From (1)

$$y' = f \text{ by differentiating}$$

$$y'' = f' = \frac{\delta f}{\delta x} + \left(\frac{\delta f}{\delta y}\right) y' \dots\dots\dots\dots\dots\dots\dots\dots\dots.. (3)$$

and the Taylor series becomes

$$y(x + h) = y(x) + hf + \frac{h^2}{2!} f' + \frac{h^3}{3!} f'' + \cdots \qquad (4)$$

Where $f', f'', f''', \dots\dots\dots\dots$ are evaluated at (x, y(x)) make the approximation

$$y(x + h) \approx y(x) + hf + \cdots \qquad (5)$$

by neglecting higher powers of h.

Introduce the iteration process, where in the last step;

We compute

$$y_1 = y_0 + hf(x_0, y_0) \dots\dots\dots\dots\dots\dots\dots\dots\dots\dots.. (6)$$

Which is approximately y(x_1) = y(x_0 + h). IN the 2nd step, we compute

$$y_2 = y_1 + hf(x_1, y_1) \dots\dots\dots\dots\dots\dots\dots\dots\dots.. (7)$$

which is approximately

y(x_2) = y(x_0 + 2h) etc.

In general, we write

$$y_{n+1} = y_n + hf(x_n, y_n) \dots\dots\dots\dots\dots\dots\dots\dots\dots (8)$$

Apply the Euler method to the initial value problem

$$y' = x + y, \quad y(0) = 0$$

Choosing h = 0.2 & multiplying y_1, y_2,…..,y_n.

Hence f(x, y) = x + y and we see that equ. (8) becomes

$$y_{n+1} = y_n + 0.2(x_n + y_n)$$

N	x_n	y_n	$0.2(x_n + y_n)$	Error	Exact values
0	0.0	0.00	0.000	0.000	0.000
1	0.2	0.00	0.040	0.021	0.021
2	0.4	0.04	0.088	0.052	0.092
3	0.6	0.128	0.146	0.074	0.222
4	0.8	0.274	0.215	0.0152	0.426
5	1.0	0.489		0.229	0.718

An indication of the accuracy of the value may be obtained by applying the Euler method again with 2h = 0.4 and comparing approximation they differ by 0.04 at $x_0 = 0.4$ and 0.110 at $(x_0) = 0.8$ since the error is of order h^2, a switch from h to 2h corresponds to a multiplication by $2^2 = 4$, but since we need twice as many steps as before, the error we have will be multiplied by 4, hence those differences indicate the size of the error.

THE EULER-CAUCHY METHOD

The corresponding formulas can be represented in such a form that a computation of the derivatives of f(x, y) is avoided. So an improved Euler-Cauchy method is an example.

In each step of this method, we first compute the auxiliary;

$y^*_{n+1} = y_n + hf(x_n, y_n)$

and then the new value:

$$y_{n+1} = y_n + \frac{1}{2}h[f(x_n, y_n) + f(x_{n+1}, y^*_{n+1})]$$

Cauchy – Euler method is a predictor corrector method.

The improved Euler method (Euler-Cauchy method) is a 2nd order method. The truncation error is of order h^3.

Exercise: Apply the E.C method to solution of equation (1)

CHOICE OF STEP VALUE h

(a) The value of h should not be too small because otherwise the round-off error and truncation error becomes too large.

(b) Also h should not be too large because large h implies large truncation error.

2.0 RUNGE-KUTTA METHOD

Is of greater accuracy and better practicable method than the other two methods discussed. Let A_n, B_n, C_n and D_n and the new value y_{n+1}.

Algorithm for Runge-Kutta method

Given an initial problem

$$y' = f(x, y), \qquad y(x_0) = y_0$$

where h is such that the problem has a unique solution y(x) on some interval containing x_0. Also, given h & n.

for n = 0, 1, ………., n-1, do

$$A_n = hf(x_n, y_n)$$

$$B_n = hf(x_n + \frac{1}{2}h, y_n + \frac{1}{2}A_n)$$

$$C_n = hf(x_n + \frac{1}{2}h, y_n + \frac{1}{2}B_n)$$

$$D_n = hf(x_n + h, y_n + C_n)$$

$$y_{n+1} = y_n + \frac{1}{6}(A_n + 2B_n + 2C_n + D_n)$$

then y_{n+1} is an approximation to $y(x_{n+1})$

where

$$x_{n+1} = x_0 + (n + 1)h$$

Runge-Kutta method is a 4th order method.

3.0 EXPANSION OF INIFINITE SERIES

Expansion of infinite series makes possible the numerical solution of many important physical problems. The solution of certain differential equations that occur frequently in the mathematical representation of many physical problem are expressed in terms of infinite series.

Definitions

Sequence: - A sequence is a succession of terms formed according to some fixed rules or laws

e.g. 1, 4, 9, 16, 25 & x, x^2, $\frac{x^3}{1x\,2}$, $\frac{x^4}{1x\,2\,x\,3}$ etc.

Series: - A series is the indicated sum of the terms of a sequence i.e. 1 + 4 + 9 + 16 + 25 and $x +$

$x^2 + \frac{x^3}{1\,x\,2} + \frac{x^4}{1\,x\,2\,x\,3}$. If the number of terms is limited, the sequence of the series is said to be finite. The general term or nth term is the expression that indicates the law of formation of the terms of the series e.g. the series 1 + 4 + 9 + 16 + 25 =

$$\sum_{i=0}^{n} n^2 \Rightarrow n \quad ^{th}terms\ is\ n^2$$

and

$$x + x^2 + \frac{x^3}{1\,x\,2} + \frac{x^4}{1\,x\,2\,x\,3} = \sum_{i=1}^{n} \frac{nx^n}{n!}$$

Where n! = 1 x 2 x 3 x 4.... x (n-1)n

nth term $\Rightarrow nx^n = \frac{hx^n}{n!}$

3.1   POWER SERIES

This is a series of the form:

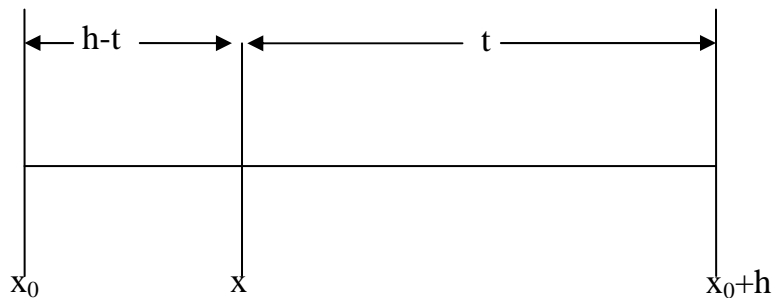S = a_0 + a_1x + a_2x^2+ ..... + a_nx^n

Where the coefficients a_0, a_1, a_2, ... are independent of x e.g. the Taylor's series.

3.1.1   The Taylor's Series is a method of expanding a given function f(x) into a power series.

Consider

$$\int_{x_0}^{x_0+h} f'(x)dx = f(x_0 + h) - f(x_0) \dots\dots\dots\dots\dots\dots\dots\dots \quad (3.1)$$

We can express the above in terms of x and t.

Let us change the variable of integration from x to t by means of the equation

$$x = (x_0 + h) - t$$

Substituting into equation (3.1) gives

$$\int_{x_0}^{x_0+h} f'(x)dx = -\int_h^0 f'(x_0 + h - t)dt = \int_0^h f'(x_0 + h - t)dt \dots \dots \dots \dots . (3.2)$$

Consider

$$\int_{x_0}^{x_0+h} f'(x)dx = f(x_0 + h) - f(x_0) \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots . . \quad (3.3)$$

We can integrate the above by part and substituting, we have

$$\int_0^h f'(x_0 + h - t)dt = [tf'(x_0 + h - t]_0^h + \int_0^h tf''(x_0 + h - t)dt$$

$$= hf'(x_0) + \int_0^h tf''(x_0 + h - t)dt \dots \dots \dots \dots \dots \dots \dots (3.4)$$

After n integrations by parts, we have

$$\int_0^{x_0+h} f'(x)dx = hf'(x_0) + \frac{h^2}{2!}f''(x_0) + \frac{h^3}{3!}f'''(x_0) + \cdots + \frac{h^n}{n!}f^n(x_0)$$

$$+ \int_0^h \frac{t^n}{n!}f^{n+1}(x_0 + h - t)dt$$

$$\approx f(x_0 + h) - f(x_0)$$

The last integral can be written in the form:

$$\int_0^h \frac{t^n}{n!}\varphi(t)dt = \frac{1}{n!}\int_0^h t^n\varphi(t)dt = I \dots \dots \dots \dots \dots \dots \dots (3.7)$$

Where $\varphi(t) = f^{(n+1)}(x_0 + h - t) \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots$ (3.8)

The integral I may be regarded as representing the area under the curve $y = t^n\varphi(t)$ from the point $t = 0$, $t = h$. If $\varphi(t)$ is a continuous function of t^n, there will be some points such that $0 < t_0 < h$ for which we shall have

$$I = \frac{1}{n!}\int_0^h t^n\varphi(t)dt = \frac{\varphi(t_0)}{n!}\int_0^h t^n dt \dots \dots \dots \dots \dots \dots \dots . (3.9)$$

Which gives

$$\frac{h^{n+1}}{(n+1)!} \varphi(t_0) = \frac{h^{n+1}}{(n+1)!} f^{n+1}(x_0 + \theta h) \quad 0 < \varphi < 1 \quad \text{......................} (3.10)$$

Where $\theta h = h - t_0$

Hence

$$f(x_0 + h) = f(x_0) + \frac{h}{1!} f'(x_0) + \frac{h^2}{2!} f''(x_0) + \cdots + \frac{h^n}{n!} f^n(x_0)$$

$$+ \frac{h}{(n+1)!} f^{(n+1)}(x_0 + \theta h) \quad 0 < \theta < 1 \text{......................} (3.11)$$

Equation (3.11) is the Taylor's formular with the Langragian form of the remainder. In derivation of Taylor's formular, it was assumed that f(x) possesses a continuous nth derivative. The term $R_{n+1} = \frac{h^{n+1}}{(n+1)!} f^{(n+1)}(x_0 + \theta h)$ is called the remainder after (n+1) terms. It may happen that f(x) possesses derivates of all orders and that the $\lim_{n \to \infty} R_{n+1} = 0$. In that case, we have the convergent infinite series:

$$f(x_0 + h) = f(x_0) + \frac{h f'(x_0)}{1!} + \cdots + \frac{h^n f^n(x_0)}{n!} + \cdots \qquad (3.12)$$

If we place $x_0 = 0$ and h = x, we obtain

$$f(x) = f(0) + \frac{x f'(0)}{1!} + \frac{x^2 f''(0)}{2!} + \cdots + \frac{x^n f^{(n)}(0)}{n!} \text{............}. (3.13)$$

(3.13) is called the Maclaurin series.

<u>Example (1)</u>: Obtain the Maclaurin series expansions of the function $f(x) = e^x$.

<u>Solution</u>: using equ. 3.13

$$f(0) = 1, \qquad f'(0) = 1, \text{......} f^{(n)}(0) = 1$$

$$\therefore e^x = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \frac{x^4}{4!} + \cdots + \frac{x^n}{n!}$$

<u>Example (2)</u>: Obtain the Maclaurin series expansion for f(x) = cosx

<u>Solution</u>:

$$f(0) = 1, \qquad f'(0) = 0, \quad f''(0) = -1, \qquad f'''(0) = 0$$

$$\therefore cosx = 1 - \frac{x^2}{2!} + \frac{x^4}{4!} - \frac{x^6}{6!} + \cdots \frac{(-1)^{n-1} x^{2n-2}}{(2n-2)!} + \cdots$$

This converges for all values of x

SST: Try for $f(x) = e^{ix}$

3.1.2   The Binomial Series

If we consider the function f(x) = (1+x)ⁿ and expand it using Maclaurin series in powers of x, we have:

$$
\left.
\begin{aligned}
f'(x) &= n(1-x)^{n-1} \\
f''(x) &= n(n-1)(1+x)^{n-2} \\
f'''(x) &= n(n-1)(n-2)(1+x)^{n-3} \\
f^r(x) &= n(n-1)(n-2)(n-3)\dots\dots(n-r+1)(1+x)^{n-r}
\end{aligned}
\right\} \quad 3.14
$$

Substituting (3.14) into (3.13) we have

$$
(1+x)^n = 1 + nx + \frac{n(n-1)}{2!}x^2 + \frac{n(n-1)(n-2)}{3!}x^3 + \cdots
$$
$$
+ \frac{n(n-1)(n-2)\dots(n-r+1)}{r!}x^r \quad \dots\dots\dots\dots (3.15)
$$

This series is convergent if $|x| < 1$ and divergent when $|x| > 1$. If n is a positive integer, the series is infinite.

We may also write $(a+b)^n = a^n(1+x)^n$ if x = b/a

i.e.

$$
(a+b)^n = a^n + na^{n-1}b + \frac{n(n-1)a^{n-2}b^2}{2!} + \cdots + \frac{n!\, a^{n-r}b^r}{(n-r)!\, r!}
$$

4.0   NUMERICAL DIFFERENTIAL & INTEGRATION

4.1   DIFFERENTIATION

It happens very frequently in practical applications that one encounters a differential equation describing some physical systems which cannot be readily solved by analytical methods. The reason being that it is usually either too complex or non-linear and cannot be solved analytically.

If f(x) is a function and $f'(x) = \frac{df}{dx}$, we can use Taylor's expansion to obtain a relation which gives a value for f(x) at a point x + h and x − h as follows:

$$
f(x+h) = f(x) + hf'(x) + \frac{h'}{2!}f''(x) + \frac{h^2}{3!}f'''(x) + \frac{h^4}{4!}f^{(iv)}(x) + \cdots \qquad (4.1)
$$

$$
f(x-h) = f(x) - hf'(x) + \frac{h^2}{2!}f''(x) - \frac{h^3}{3!}f'''(x) + \frac{h^4}{4!}f^{(iv)}(x) + \cdots \qquad (4.2)
$$

If we subtract (4.2) from (4.1), we get the 1ˢᵗ derivative

$$f(x + h) - f(x - h) = 2hf'(x) + \frac{2h^3}{3!}f'''(x) + \frac{2h^5}{5!}f^{(v)}(x) \qquad (4.3)$$

If h is very small so that $h \to 0$, we may neglect the terms h^3 and h^5 above so that

$$f(x + h) - f(x - h) \approx 2hf'(x)$$

$$\therefore f'(x) = \frac{f(x + h) - f(x - h)}{2h} \qquad (4.4)$$
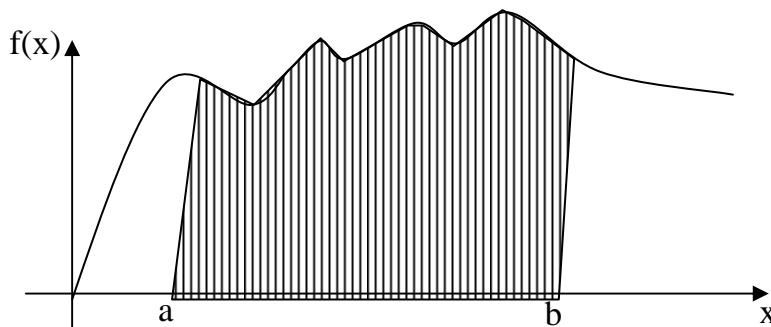
Which is the Stirling's formula, where h is the step size.

To get the 2nd derivate, add (4.1) and (4.2):

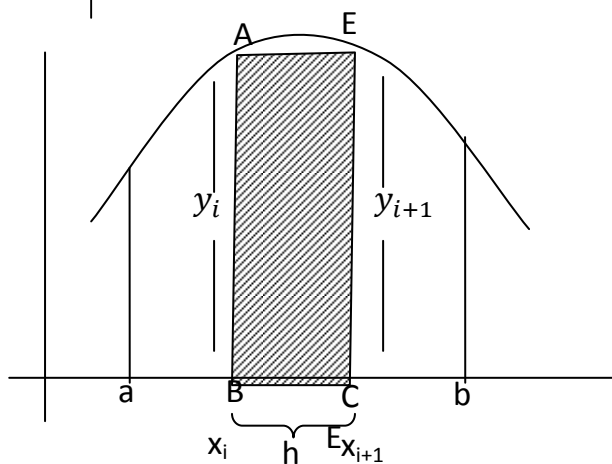$$f(x + h) + f(x - h) = 2f(x) + \frac{2h^2}{2!}f''(x) + \frac{2h^4}{4!}f^{(iv)}(x) \qquad (4.5)$$

4.2   INTEGRATION

Suppose a function f is positive in an interval D = {a ≤ x ≤ b}. We seek the area under the curve y = f(x) between x = a and x = b. This area is shaded in fig. Below and is equal to

$$\int_a^b f(x)dx$$

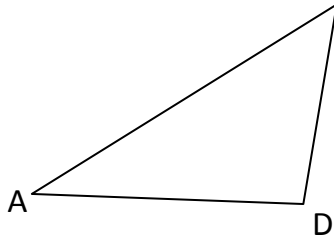The interval has been divided into n strips; h being the width of the strips

Lenghtab = nh

$y_i = f(x_i)$

$y_{i+1} = f(x_{i+1})$

Area of rectangle ABCD = y_ih.

Area of ☐ ABCD = $y_{i=h}$

$$\text{Area of } \triangle ADE = \frac{1}{2}h(y_{i+1} - y_i)$$

Area of the total strip ABCE is

$$A = y_i h + \frac{1}{2}h(y_{i+1} - y_i) = y_i h + \frac{1}{2}y_{i+1}h - \frac{1}{2}y_i h$$

$$= \frac{1}{2}h(y_i + y_{i+1}) \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots \quad (4.7)$$

For a single strip, area $= \frac{h}{2}(y_i + y_{i+1})$

$$I_i = \int_{x_i}^{x_{i+1}} f(x)dx = \frac{h}{2}(y_i + y_{i+1})$$

$$= h\left[\frac{(y_0 + y_n)}{2} + y_1 + y_2 + y_3 + \cdots + y_{n-1}\right] \dots \dots \dots \dots \dots \dots \quad (4.8)$$

Equation (4.8) is called the trapezoidal rule. There is error due to the truncation of the small triangles.

There is another numerical integration method called the Simpson's rule. Consider a parabolic function f(x) = $y(x) = y_0 + \propto x + \beta x^2$ shown below
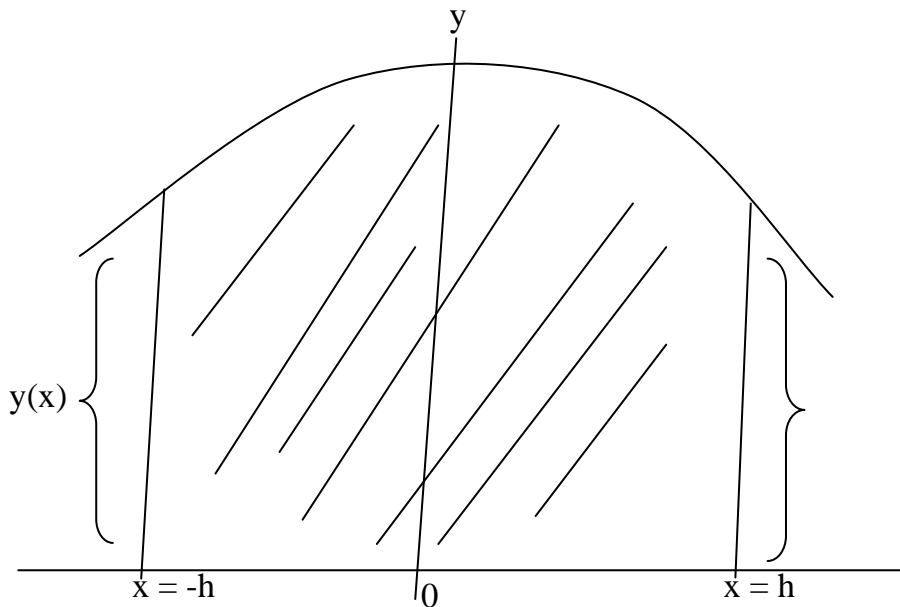
At x = 0, y(0) = f(0) = y_0

At x = -h, y(-h) = $y_0 - \alpha h + \beta h^2$ ------------------------------------- (4.9)

At x = +h, y(h) = $y_0 + \alpha h + \beta h^2$ ------------------------------------- (4.10)

Adding (4.9) and (4.10 we have

$$y(h) + y(-h) = y(-h) + y(h) = 2y_0 + 2\beta h^2$$

$$2\beta h^2 = y(-h) + y(h) - 2y_0$$

$$\beta h^2 = \frac{y(-h) + y(h)}{2} - y_0 \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots (4.11)$$

$$= 2y_0 h + 0 + \frac{2\beta h^3}{3} = 2h\left(y_0 + \frac{\beta h^3}{3}\right) \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots (4.12)$$

Substitute (4.11) into (4.12) to get

$$I = 2h\left[y_0 + \frac{1}{3}\left(\frac{y(-h) + y(h) - 2y_0}{2}\right)\right]$$

$$I = \frac{h}{3}[y(-h) + y(h) + 4y_0]$$

For n even strips, area of strips from n = 0 to n = 2 is

$$I_1 = \frac{h}{3}[y_0 + y_2 + 4y_1]$$

Area of strips from n = 2 to n = 4

$$I_2 = \frac{h}{3}[y_2 + y_4 + 4y_3]$$

Area of strips from n = 4 to n = 6

$$I_3 = \frac{h}{3}[y_4 + y_6 + 4y_5]$$

Finally, area of strips from n-2 to n will be

$$I_{\frac{n}{2}} = \frac{h}{3}[y_{n-2} + y_n + 4y_{n-1}]$$

Adding all the areas of the strips, we get

$$I = \int_a^b f(x)dx$$

$$= \frac{h}{3}\left[y_0 + y_n + 4\sum odd\ terms\ + 2\sum even\ terms\right] \dots \dots \dots \dots \dots (4.13)$$

Example 1: Perform the following integration using Simpson's rule and trapezoidal rule. In each case use grid size of 0.2. Compare your results with the exact solution. The expression is

$$\int_0^2 x^2 e^{-x}dx$$

Solution

$$h = \frac{b-a}{n} = 0.2 \quad \Rightarrow \quad n = 10$$

$$y(x) = f(x) = x^2 e^{-x}$$

$$y_0 = y(0) = 0$$

$$y_1 = y(0.2) = (0.2)^2 e^{-0.2}$$

$$y_2 = y(0.4) = (0.4)^2 e^{-0.4}$$

$$y_{10} = y(2) = 4e^{-2}$$

$$I = \int_0^2 x^2 e^{-x} dx$$

$$= \frac{0.2}{3}[(0 + y_{10}) + 4(y_1 + y_3 + y_5 + y_7 + y_9) + 2(y_2 + y_4 + y_6 + y_8)]$$

=

Example 2: The Debye function is encountered in the theory of specific heat of solids at constant volume. The function is expressed as

$$D(x) = 3x^{-3} \int_0^x \left(\frac{y^3}{e^y - 1}\right) dy \quad or \quad D(x) = 3x^{-3} \int_0^x f(y) dy.$$

Evaluate this integral for x = 10.0 using Simpson's rule. You may use the grid size as 0.5

4.3   ALGORITHM

Algorithm is a finite sequence of rules for performing computations on a computer such that at each instance the rule determines exactly what the computer has to do next. These rules include a "stopping rule" that makes the computer stop so it cannot run - on indefinitely. A useful and good algorithm is one that is stable. Small changes in the initial data should give only corresponding small changes in the final result. However, if small changes in the initial data produces large changes in the final results, the algorithm is unstable.

4.3.1   Algorithm for Simpson's Rule

x_j, f_j, j = 0, 1, ..., 2m

$J = \int_a^b f(x) dx$ from given values of $f_j = f(x_j)$ at equidistant.

$x_0 = a$, $x_1 = x_0 + h$, ... $x_{2m} = x_0 + 2mh$

Where h $= \frac{b-a}{2m}$ $\qquad (n = 2m)$

STEPS

Compute $S_0 = f_0 + f_n \ (f_{2m})$

$S_1 = f_1 + f_3 + f_5 + \dots + f_{n-1}$

$S_2 = f_2 + f_4 + \dots + f_{n-2}$

$h = \dfrac{b-a}{2m}$

$\hat{J} = \dfrac{h}{3}(S_0 + 4S_1 + 2S_2)$

Output $\hat{J}$

STOP

4.4   ERRORS OF NUMERICAL RESULTS

Final results of computations of unknown quantities generally are approximations. That is they are not exact but involves errors. Such an error may result from a combination of the following effects.

Round off errors – resulting from rounding off figures

Experimental errors – arises as a result o given data probably from measurement.

Truncating errors – resulting from truncating i.e. prematurely breaking off e.g. if a given series is replace by the sum of its 1st few terms.

These errors depend on the computational method used and must be dealt with individually for each method.

4.4.1   Formulas for Errors

If $\tilde{a}$ is an approximate value of a quantity whose value is a, we call the difference error t. The error t is given by

$$t = a - \tilde{a} \ \dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots. (4.1)$$

The exact value is thus

$$a = \tilde{a} + t$$

i.e. True value = Approximation + error

Example

(i)   If a = 10.2 and $\tilde{a}$ = 10.5 $\therefore$ t = -0.3

(ii)   If a = 1.82 and $\tilde{a}$ = 1.60 $\therefore$ t = 0.22

The relative error t_r of $\tilde{a}$ can be defined as

$$t_r = \frac{t}{a} = \frac{a - \tilde{a}}{a} = \frac{Error}{True\ value} \ \dots\dots\dots\dots\dots\dots\dots\dots\dots. (4.2)$$

Here a ≠ 0

Eq. (4.2) appears useless since a is unknown. However if $|t| \ll |\tilde{a}|$, then we can use $\tilde{a}$ instead

of a and obtain $t_r \approx \dfrac{t}{\tilde{a}}$.. (4.3)

(4.3) still appears problematic because t is unknown. If it were known, we would have obtained

$a = \tilde{a} + t$, but this can be obtained in practice from a bound for $\tilde{a}$ i.e. a number β such that

$|t| \le \beta$, hence

$$|a - \tilde{a}| \le \beta \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots (4.4)$$

Where β is limiting absolute error. The limiting absolute error of an approximate number is any

number not less than the absolute error of that number. It tells us how far away from our

computed $\tilde{a}$ the unknown a can at most lie. Similarly for the relative error, an error bound is a

number β_r such that

$$|t_r| \le \beta_r.$$

Thus we have

$$\left| \frac{a - \tilde{a}}{a} \right| \le \beta_r \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots (4.5)$$

Where β_r is the limiting relative error and is defined as any number less than the relative error

of that number.

4.4.2   Error Bound for the Trapezoidal Rule

Error for a given function f(x) is given by

$t_n(x) = f(x) − P_n(x)$

$$= (x − x_0)(x − x_1) \ldots (x − x_n)\frac{f^{(n+1)}(t)}{(n+1)!} \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots (4.6)$$

With n = 1, we have

$$f(x) − p_1(x) = (x − x_0)(x − x_1)\frac{f'''(t)}{2!}$$

With suitable t depending on x, between x_0 and 1. Integration over x from $a = x_0$ to $x_1 = x_0 + h$

gives

$$\int_{x_0}^{x_0+h} f(x)dx + \frac{h}{2}[f(x_0) + f(x_1)]$$

$$= \int_{x0}^{x_0+h} (x − x_0)(x − x_0 − h)\frac{f''(t(x))}{2}dx \ldots \ldots. (4.7)$$

Setting $x - x_0 = v$ and applying the mean value theorem of integral calculus, which we can use because $(x - x_0)(x - x_0 - h)$ does not change sign, we find that the right side equals

$$\int_0^h v(v - h)dv \frac{f''(\tilde{t})}{2} = \left(\frac{h^3}{3} - \frac{h^2}{2}\right)\frac{f''(\tilde{t})}{2} = \frac{-h^3}{12}f''(\tilde{t}) \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots (4.8)$$

Where $\tilde{t}$ is a suitable value between x_0 and x_1. Hence the error t of trapezoidal rule is the sum of n such contribution from the n subinterval.

Since $h = \frac{b-a}{n}$, we thus obtain the total error

$$t = \frac{-(b-a)^3}{12n^2}(\tilde{t}) \quad \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots (4.9)$$

where $\tilde{t}$ is suitable value between a and b.

Finally, error bounds are now obtained by taking from f'' the largest value M_2 and smallest value M^*_2 in the interval of integration obtaining

$$KM_2 \leq t \leq KM_2^* \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots (4.10)$$

Where $K = \frac{-(b-a)^3}{12n^2} \quad \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots (4.11)$

Example: Evaluate

$$J = \int_0^1 e^{-x^2} dx \qquad with\ n = 10$$

Solution

J	x_j	x_j^2	$e^{-x_j^2}$
0	0	0	1.00000
1	0.1	0.01	0.990050
2	0.2	0.04	0.960789
3	0.3	0.09	0.91393
4	0.4	0.16	0.85214
5	0.5	0.25	0,77881
6	0.6	0.36	0.69768
7	0.7	0.49	0.61263

8	0.8	0.64		0.52729
9	0.9	0.81		0.444858
10	1.0	1.00	0.367879	
			1.367879	6.778167

$$I = h\left[\left(\frac{y_0+y_n}{2}\right) + y_1 + y_2 + y_n + \cdots + y_{n-1}\right]$$

$$h = \frac{b-a}{n}$$

$$= 0.1[0.5 \times 1.367879 + 6.778167]$$

$$= \frac{1-0}{10}$$

$$= 0.746211$$

Error estimate

$$= 0.1$$

$$f''(0) = 2(2x^2 - 1)e^{-x^2}$$

If $0 < x < 1$, $f''(x) > 0$

$M_2 = f''(1) = 0.735759$

$M*_2 = f''(0) = -2$

$K = \dfrac{1}{-1200}$

$$\Rightarrow -0.000614 \leq t \leq 0.001662$$

$$0.746211 - 0.00614 \leq J \leq 0.746211 + 0.001667$$

$$0.745597 \leq J \leq 0.747878$$

4.4.3 Bounds for the Error t_s

Assuming the 4th derivative of f exist and is continuous in the interval of integration, the result is

$$CM_4 \leq t_s \leq CM_4^* \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots (4.12)$$

Where $C = \dfrac{-(b-a)^5}{180(2m)^4}$ $\ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots (4.13)$

M_4 and $M*_4$ are the largest and the smallest value of the 4th derivative of in the interval of integration.

Example: Evaluate

$$J = \int_0^1 e^{-x^2}\, dx$$

2m = 10, h = 0.1

<u>Using Simpson's Rule</u>

J	x_j	x_j^2	$e^{-x_j^2}$		
0	0	0	1.00000		
1	0.1	0.01		0.990050	
2	0.2	0.02			0.960789
3	0.3	0.09		0.91393	
4	0.4	0.16			0.852144
5	0.5	0.25		0.778801	
6	0.6	0.36			0.697676
7	0.7	0.49		0.612626	
8	0.8	0.64			0.527292
9	0.9	0.81		0.444858	
10	1.0	1.00	0.367879		
			1.367879	3.740266	3.037901

$$y = \frac{0.1}{3}[(1.367879 + 4(3.740266) + 2(3.037901)]$$

= 0.746825

Estimate of error

By differentiating 4 times, we have

$$f^{iv}(x) = 4(4x^4 - 12x^2 + 3)e^{-x^2}$$

The largest value occur at x = 0

Smallest value occur at x = x* = 2.5 + 0.5$\sqrt{10}$

∴ $M_4 = f^{iv}(0) = 12$, $M*_4 = f^{iv}(x*) = -7.359$

$2m = 10$, $b - a = 1 \Longrightarrow C = \dfrac{-1}{(18000000)}$

$= -0.00000056$

$-0.0000007 \leq t_z \leq 0.00000056$

4.5   GAUSIAN INTEGRATION FORMULAR

The integration formulars discussed so far involve function values for equidistant x values exceeding a certain degree. More generally, we may set

$$\int_{-1}^{1} f(x)dx \approx \sum_{j=1}^{n} A_j f_j \left(f_j > f(x_j) \right) \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots \quad (4.14)$$

and determine the second constants

A_j, ..., A_n, x_1, ..., x_n so that equ. (4.14) gives exact results for polynomials of degree K as high as possible. Since 2n is the number of coefficients of a polynomial of degree n-1, it follows that $k \leq 2n-1$.

Gauss has shown that exactness for polynomials of degree not exceeding 2n-1 (instead of n-1 or n) can be obtained iff the values x_1, ...,x_n are the end zeroes of the Legendre Polynomial $P_n(x)$ where $P_0 = 1$, $P_1(x) = x$, $P_2(x) = \frac{1}{2}(3x^2-1)$, $P_3(x) = \frac{1}{2}(5x^3-3x)$

$$P_n(x) = \sum_{m=0}^{m} \frac{(-1)^m (2n - 2m)!}{2^n m! \, (n - m)! \, (n - 2m)!} x^{n-2m} \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots . \,(4.15)$$

$$P_n(x) = \frac{2n!}{2^n (n!)^2} x^n - \frac{(2n - 2)!}{2^n (n - 1)! \, (n - 2)!} x^{n-2} + \cdots \qquad (4.16)$$

Where $m = \dfrac{n}{2}$ or $\dfrac{n-1}{2}$

$P_4(x) = 1/8(35x^4-30x^3+3)$

$P_5(x) = 1/8(63x^5 - 70x^3 + 16x)$

and the coefficient A_j are suitably chosen. The equ. (4.14) is called a Gaussian integration formular.

We note that it can be shown that the variables can be expressed in a chosen coordinate t which could vary from -1 to +1 as follows

$$x_i = \left(\frac{b + a}{2} \right) + \left(\frac{b - a}{2} \right) t_i \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots . \,(4.17)$$

Finally, we have the following table which summarizes the results

n	Zeros(i)	t_i	A_j
2	$\pm\dfrac{1}{\sqrt{3}}$	± 0.5773502692	1
3	$\begin{cases} 0 \\ \pm\sqrt{3/5} \end{cases}$	$\begin{matrix} 0 \\ \pm 0.774596672 \end{matrix}$	$\begin{matrix} 8/9 \\ 5/9 \end{matrix}$
4	$\pm\sqrt{(15-\sqrt{20})/35}$	± 0.33999810436	0.6521451549
	$\pm\sqrt{(15+\sqrt{20})/35}$	± 0.8811363116	0.3478548451

<u>Example</u>: Evaluate

$$J = \int_0^1 e^{-x^2}\,dx$$

With the Gaussian formular for n = 3 from 0 to 1 into an integral -1 to 1

<u>Solution</u>: We use equ. (4.17) to obtain

x = ½(t + 1)

and dx = $\dfrac{1}{2}dt$

Thus

$$\int_0^1 e^{-x^2}\,dx = \int_{-1}^1 \frac{1}{2}e^{\left(-\frac{1}{4}(t+1)^2\right)}\,dt$$

$$I \approx \frac{1}{2}\left[\frac{8}{9}e^{-\frac{1}{4}} + \frac{5}{9}e^{\left(-\frac{1}{4}\left(1+\frac{\sqrt{3}}{5}\right)^2\right)} + \frac{5}{9}e^{\left(-\frac{1}{4}\left(1-\frac{\sqrt{3}}{5}\right)^2\right)}\right]$$

The Gaussian integration formula has the advantage of high accuracy. Its disadvantage is the irregular spacing of $x_i, \dots, x_n$ and the somewhat the inconvenience values of the coefficients. However this is not essential if $f(x_j)$ are also computed (not taking from table as we have done or obtain from an experiment in which the x_j can be set once and for all.

Where

$$k_0 = f(x_n, y_n$$

$$k_1 = f(x_n + \frac{1}{2}h, y_n + \frac{1}{2}hk_0)$$

$$k_2 = f(x_n + \frac{1}{2}h, y_n + \frac{1}{2}hk_1)$$

$$k_3 = f(x_n + h, y_n + hk_2)$$

$$y_{n+1} = y_n + \frac{h}{6}\left[k_1 + 2\left(1 - \frac{1}{\sqrt{2}}\right)k_2 + \left(1 + \frac{1}{\sqrt{2}}\right)k_3 + k_4\right] \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots (12)$$

Where

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

$$k_2 = f(x_n + \frac{1}{2}h, y_n + \frac{1}{2}hk_1)$$

$$k_3 = f\left(x_n + \frac{1}{2}h, y_n + \left(-\frac{1}{2} + \frac{1}{\sqrt{2}}\right)hk_1 + \left(1 - \frac{1}{\sqrt{2}}\right)hk_2\right)$$

$$k_4 = f\left(x_n + h, y_n - \frac{1}{\sqrt{2}}hk_2 + \left(1 + \frac{1}{\sqrt{2}}\right)hk_3\right) \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots (13)$$

Select last equation as pivot equation

$$-3x_1 + 2x_2 + x_3 = 1$$

$$12x_2 + x_3 = 37$$

$$\frac{37}{6}x_3 = \frac{37}{6}$$

$$\therefore \quad x_3 = 1 \text{ and so on.}$$

5.0 NUMERICAL SOLUTION OF ORDINARY DIFFERENTIAL EQUATIONS

5.1 EULER'S METHOD.

The numerical methods are for equations that cannot be solved analytically or equations for which the solutions in terms of formulas are so complicated that one often prefers to compile a table of values by applying a numerical method to such an equation .

A differential equation of the 1st order is of the form

$$F(x, y, y') = 0$$

and often it will be possible to write the equation in the exclusive form

$$y' = f(x, y)$$

An initial value problem consist of a differential equation and a condition the solution must satisfy (or several conditions reffering to the same value of x, if the equation is of the higher order)

$$y' = f(x, y), \quad y(x_0) = y_0 \qquad (5.1)$$

$$x_1 = x_0 + h, \quad x_2 = x_0 + 2h, \quad x_3 = x_0 + 3h, \dots \dots \dots \dots \dots \dots$$

The soluton of the equation (7.1) can be obtained using Taylor's series as well i.e

$$y(x + h) = y(x) + hy'(x) + \frac{h^2}{2} y''(x) + \cdots \dots \dots \qquad (5.2)$$

for small h, h^2, h^3, …… are very small . Thus,

$$y(x + h) \approx y(x) + hy'(x) \approx y(x) + hf(x, y)$$

To carry out the solution we follow the steps below :

i. $y_1 = y_0 + hf(x_0, y_0)$
   $y(x_1) = y_0(x_0 + h)$

ii. $y(x_2) = y(x_0 + 2h)$

In general

$$y_{n+1} = y_n + hf(x_n, y_n) \qquad n=0,1,2,\dots\dots\dots\dots\dots\dots\dots\dots \qquad (5.3)$$

Eqn(7.3) is simply called the Euler method. The omission of the further terms in eqn(7.2) causes an error which is called the **truncation error** of the method.

For small h , the 3rd and higher powers of h will be small compared with h^2 in the 1st neglected term in (7.2) and we therefore say that the truncation error per step (local truncation error) is of order h^2. In addition, there are round off errors in these and other methods which may affect the accuracy of the values $y_1, y_2, y_3, \ldots\ldots$ etc more and more as n increases.

Example 7.1:   Apply the Euler method to the following initial value problem choosing h=0.3 and computing $y_1,\ldots\ldots\ldots,y_5$.

$$y' = x + y \qquad\qquad y(0) = 0$$

Solution

$$f(x, y) = x + y$$

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

$$i.e \ \ y_{n+1} = y_n + 0.2(x_n + y_n)$$

for n=0, x_0 = 0, y_0 = 0

N	x_n	y_n	$0.2(x_n+y_n)$	Exact values	Error
0	0.0	0.000	0.000	0.000	0.000
1	0.2	0.000	0.040	0.021	0.019
2	0.4	0.040	0.088	0.092	0.052
3	0.6	0.128	0.146	0.222	0.094
4	0.8	0.274	0.215	0.426	0.152
5	1.0	0.489		0.718	0.229

N.B: Exact solution is $y(x) = e^x - x - 1.$

5.2   **LINEAR DIFFERENTIAL EQUATION**

$$y' + p(x)y = r(x) \text{------------------------}^{(7.4)}$$

If $r(x) = 0 \Rightarrow$ (7.4) is homogenous else (7.4) is non-homogenous.

For homogenous equations,

$$y' + p(x)y = 0$$

i.e $\quad \dfrac{dy}{y} = -p(x)dx$

$\Rightarrow \ln|y| = -\int p(x)dx + c$

So that the solution is

$$y(x) = ce^{-\int p(x)dx} \text{------------------------} \text{(7.5)}$$

For non-homogenous equations

$$(P_y - r)dx + dy = 0$$

$$Pdx + Qdy = 0$$

Where P=P_y – r , Q = 1

$$\dfrac{1}{F}\dfrac{dF}{dx} = P(x)$$

$$F(x) = e^{\int pdx}$$

$$\Rightarrow e^{\int pdx}(y' + p_y) = (e^{\int pdx}rdx + c$$

Solve for y where $h = \int pdx$

$$\therefore y(x) = e^{-h}[\int e^h rdx + c]\text{.............................}\text{(5.6)}$$

Question: $\qquad$ Solve $y' - y = e^{2x}$

In practice the exact solution is unknown but an indication of the accuracy of the values can be obtained by applying the Euler method once more with step *2h* and comparing the corresponding approximation.

x_n	y_n	$0.4(x_n+y_n)$	y_n	Difference

0.0	0.000	0.000	0.000	0.000
0.4	0.000	0.160	0.040	0.040
0.8	0.160		0.274	0.1140

6.0   RUNGE-KUTTA METHODS

Euler's method requires a very small step size in order to obtain reasonable accuracy. The Runge-kutta methods attempt to avoid these problem by obtaining higher order accuracy by simply evaluating the function at selected point. To derive this type of formula a different method is used which is described in as follows:

The desired recurrence formular is of the form:

$Y_{n+1} = y_n + a_1 k_1 + a_2 k_2$ 1

Where $K_1 = hf(x_n, y_n)$ 2

$\quad K_2 = hf(x_n + \alpha h, y_n + \beta k_1)$

To find an optimum scheme the values of a_1, a_2, α, and β are sought which make equ. 1 a Taylor series.

$$y(x_{n+1}) = y(x_n) + hy'(x_n) + \frac{h^2}{2} y''(x_n) + \frac{h^3}{6} y'''(x_{n)} + 0(h^4)$$

$$= y(x_n) + hf(x_n, y_n) + \frac{h^2}{2}(f_x + f_y)_n + \frac{h^3}{6}(f_{xx} + 2f_{xy} + f_{yy}f^2 + f_x f_y + f_y^2 f)_n + 0(h^4) \dots \dots 3$$

Where +o(h^4) means plus of order h or less, all terms are evaluated at (x_n,y_n). Expanding equation 2 using taylor's series for a function of two variables,

$$\frac{k_2}{h} = f(x_n + \alpha h, y_n + \beta k_1)$$

$$= f(x_n, y_n) + \alpha h f_x + \beta k_1 f_y + \frac{\alpha^2 h^2}{2} f_{xx} + \alpha h \beta k_1 f_{xy} + \frac{\beta^2 k_1^2 f_y}{2} + 0(h^3) \dots \dots 4$$

Substituting into equation 1 using 2 gives:

$$y_{n+1} = y_n + (a_1 + a_2)hf + a_2 h^2 (\alpha f_x + \beta f f_y) + a_2 h^3 \left(\frac{\alpha^2}{2} f_{xx} + \alpha \beta f f_{xy} + \frac{\beta^2}{2} f^2 f_{yy} \right)$$
$$+ 0(h^4) \dots \dots \dots \dots \dots \dots \dots \dots \dots 5$$

Comparing the exact Taylor's series with equation 5 we find that

$$hf(x_n, y_n) = (a_1 + a_2)hf \dots \dots \dots \dots \dots \dots \dots \dots .. 6$$

$$\frac{h^2}{2}(f_x + ff_y)_n = a_2 h^2(\alpha f_x + \beta ff_y) \ldots \ldots \ldots \ldots \ldots .7$$

And

$$\frac{h^3}{b}(f_{xx} + 2f_{xy} + f_{yy}f^2 + f_xf_y + f_2^y f$$

$$= a_2 h^3 \left(\frac{\alpha^2}{2}f_{xx} + \alpha\beta ff_{xy} + \frac{\beta^2}{2}f^2 f_{yy}\right) \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots . 8$$

Rewriting 6 and 7 we have:

$$a_1 + a_2 = 1$$

$$a = \alpha = \frac{1}{2} \text{ and } a_2\beta = \frac{1}{2} \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots . 9$$

From 6 and 7 we have derived three equations with four unknowns. By examining equation 8, 5 we find that another equation cannot be defined independently of f(x,y) so we must be satisfied with obtaining agreement up to h^2. There are many solutions to equation 9, the simplest being

$$a_1 = a_2 = \frac{1}{2}$$

$$\alpha = \beta = 1$$

Thus,

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

$$= y_n + \frac{h}{2}[(f(x_n, y_n) + f(x_n + h, y_n + hf(x_n + y_{n)})] \ldots \ldots \ldots \ldots \ldots 10$$

Equation 10 is known as the second order Runge-kutta method or the improved Euler method.

Using the same approach, we can obtain higher order schemes by simply adding more terms. The most commonly used scheme is the fourth order Runge-kutta method given by

$$y_{n+1} = y_n + \frac{h}{6}(k_0 + 2k_1 + 2k_2 + k_3) + o(h^5) \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots .1$$

Where

$$k_0 = f(x_n, y_n$$

$$k_1 = f(x_n + \frac{1}{2}h, y_n + \frac{1}{2}hk_0)$$

$$k_2 = f(x_n + \frac{1}{2}h, y_n + \frac{1}{2}hk_1)$$

$$k_3 = f(x_n + h, y_n + hk_2)$$

NB: There are several other fourth-order method ascribed to kutta. Another most widely used fourth order method is the one credited to hill and is given by

$$y_{n+1} = y_n + \frac{h}{6}\left[k_1 + 2\left(1 - \frac{1}{\sqrt{2}}\right)k_2 + \left(1 + \frac{1}{\sqrt{2}}\right)k_3 + k_4\right] \dots \dots \dots \dots \dots \dots \dots \dots \dots (12)$$

Where

$$k_1 = f(x_n, y_n$$

$$k_2 = f(x_n + \frac{1}{2}h, y_n + \frac{1}{2}hk_1)$$

$$k_3 = f\left(x_n + \frac{1}{2}h, y_n + \left(-\frac{1}{2} + \frac{1}{\sqrt{2}}\right)hk_1 + \left(1 - \frac{1}{\sqrt{2}}\right)hk_2\right)$$

$$k_4 = f\left(x_n + h, y_n - \frac{1}{\sqrt{2}}hk_2 + \left(1 + \frac{1}{\sqrt{2}}\right)hk_3\right) \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots (13)$$

6.1   TRUNCATION ERROR, STABILITY AND STEP-SIZE CONTROL IN THE RUNGE-KUTTA ALGOROTHMS

In order to choose to a reasonable step size, one need some estimate of the error being committed in integrating across one step. On the other hand, the step size should small enough to achieve the required accuracy (if possible), on the other hand, it should be as large as possible in order to keep rounding errors under control to avoid an excessive number of derivatives evaluations. For nth order Runge-kutta, the local truncation is given by

$$l_t = Kh_1^{m+1} = \frac{2^m(y_{n+1,2} - y_{n+1,1})}{2^m - 1} \dots \dots \dots \dots \dots \dots \dots (14)$$

For the 4th order, m=4 and (14) becomes

$$l_t = Kh_1^5 = \frac{16}{15}(y_{n+1,2}-, y_{n+1,1})$$

Another criterion for selecting an algorithm for the solution of a differential equation with given initial conditions is stability. In general, a solution is said to be unstable if errors introduced at some stage in the calculations (for example, from erroneous initial condition

or local truncation or round off errors) are propagated without bound throughout subsequent calculations. For example, consider the equation

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

The analytic solution is:

$$y(x) = -x - 1 + [1 + x_0 + y(x_0)]e^{-x_0}e^x$$

With the initial condition y(0) = -1, the analytical solution is

$$y(x) = -x - 1$$

i.e. the exponential term in the general solution vanishes because of the Particular choice of initial condition. Inherent instability is usually associated with the equation being solved and the initial conditions specified but do not depend on the particular algorithm being used.

Depending on the equation being solved, its initial conditions, and the particular one-step method being used, another form of instability, called <u>partial instability</u>, may be observed, even when the equation is not inherently unstable. This phenomenon is related to the step size chosen.

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