



Objective

Upon completion of this chapter you will be able to:

- Solve Algebraic and Transcendental Equations by Numerical Methods.
- Perform Definite Integral using Numerical Techniques.
- Determine Solution of a Differential Equation by Numerical Methods

Introduction

There are two methods by which a mathematical problem like a differential equation, transcendental or a linear equation can be solved.

Analytical Methods:

The method by which solution of an equation can be directly obtained in terms of coefficients present in the equation.

Like Quadratic formula can be used to find the solution of a quadratic equation. An example of Integration by analytical method is shown below,

$$\int x dx = \frac{x^2}{2} = \frac{4}{2} - \frac{1}{2} = \frac{3}{2}$$

Numerical Methods:

Here, instead of directly writing the solution in terms of some formulae we perform a stepwise calculation using an algorithm to arrive at the result. These methods are more popular as they can be implemented on computers to solve a wider class of problems than what can be solved by analytical methods. Like, we do not have analytical methods for solution of a polynomial of degree 4 or more. But numerical methods work successfully on such type of problems. The only disadvantage with numerical methods is that exact solutions cannot be obtained and there is some degree of error in the solution.

Causes of Errors

The error in any numerical calculation can be quantified as, Absolute Error = | Exact Value – Approximate Value |

$$\text{Relative Error} = \left[\frac{\text{Exact} - \text{Approximate}}{\text{Exact}} \right]$$

Percentage Error =

$$\left[\frac{\text{Exact} - \text{Approximate}}{\text{Exact}} \right] \times 100\%$$

There are two main causes of Errors in There are two main causes of errors in numerical methods, which is round-off error and truncation error. Round-off error is mainly due to the limited storage capacity of the device, as we can only save the result a to few significant digits. only a few terms in an infinite series. These errors can be reduced by reducing the tolerance limit and performing more number of iterations.

Thus, there is always a trade-off between the speed of calculation and the accuracy of computation.

Solution of Algebraic and Transcendental Equations

An equation that involves trigonometric functions is called transcendental equation.

Example: $f(x) = x - \cos x = 0$

Roots of Algebraic Equation

- An algebraic equation of nth order can be represented in the form shown below:

$$f(x) = x^n + a_1x^{n-1} + a_2x^{n-2} + \dots + a_{n-1}x + a_0 = 0$$

This equation will have n roots. Certain properties of the roots of this algebraic equation are,

- Complex roots always occur in pairs. Therefore, if $(a+ib)$ is a root of the equation then $(a-ib)$ is also a root of the equation.
- Surd roots also occur in pairs. Therefore, if $a + \sqrt{b}$ then $a - \sqrt{b}$ is also the root of the equation.



Descarte's Rule of Signs

An equation $f(x)=0$ cannot have more positive roots than there are changes of sign in $f(x)$ and cannot have more negative roots than there are changes of sign in $f(-x)$.

Intermediate Mean Value Theorem (I.M.T)

Let $f(x)$ is continuous function defined in the interval $[a, b]$.

$f(a)$ and $f(b)$ having opposite signs (say $f(a)<0$, $f(b)>0$), then there exists at least one root $f(x)=0$ in the interval $[a, b]$.

Example : $f(x) = x^3 - 4x - 9 = 0$ $[2, 3]$

$$f(2) = 2^3 - 4 \times 2 - 9 = -9 < 0$$

$$f(3) = 3^3 - 4(3) - 9 = 6 > 0$$

Since $f(2) < 0$ and $f(3) > 0$. So at least one root of $x^3 - 4x - 9 = 0$ is in $[2, 3]$

Bisection Method

Let $f(x)$ is continuous function defined in $[a, b]$

1. Let $f(a) < 0$ and $f(b) > 0$

Using IMT there exists at-least one root $f(x) = 0$ in $[a, b]$

2. Let x_1 is first approximation root of $f(x) = 0$ and $x_1 = \frac{a+b}{2}$

Case 1: If $f(x) = 0$ then x_1 is root, stop the process

Case 2: If $f(x_1) > 0$, then a root of $f(x) = 0$ lies in $[x_1, b]$ then compute x_2 using $x_2 = \frac{x_1 + b}{2}$

Case 3: If $f(x_1) < 0$, then a root of $f(x) = 0$ lies in $[a, x_1]$ then compute x_2 using $x_2 = \frac{a + x_1}{2}$. The

length of new interval $[a_1, x]$ or $[x_1, b]$ is exactly

half of the previous interval i.e. $\frac{b-1}{2}$

Continue the above process until the desired accuracy of root is found. After, n iterations

the length of the interval will be $\frac{b-1}{2^n}$
If $\frac{b-a}{2^n} \leq \varepsilon$ where ε is a small positive number

indicating the desired accuracy of root then we will stop the process.

So, the number of steps required to achieve

a desired accuracy will be, $n \geq \frac{\log_e \frac{b-a}{\varepsilon}}{\log_e 2}$

Solved Examples

Example: Find x_2 and x_3 using bisection, where

$$f(x) = x^3 - 4x - 9 = 0 \text{ in } [2, 3]?$$

Solution: $f(2) = -9 < 0$

$$f(3) = 6 > 0$$

$$\text{Let } x_1 = \frac{a+b}{2} = \frac{2+3}{2} = 2.5$$

$$\text{Now } x_2 = \frac{x_1 + b}{2} = \frac{2.5 + 3}{2} = 2.75$$

$$\text{Now } x_2 = \frac{x_1 + b}{2} = \frac{2.5 + 3}{2} = 2.75$$

$$f(x_2) = (2.75)^3 - 4(2.75) - 9 = 0.7069 > 0$$

$$\therefore x_3 = \frac{x_1 + x_2}{2} = \frac{2.5 + 2.75}{2} = 2.625$$

$$x_3 = 2.62; \quad x_2 = 2.75 \text{ \& } x_3 = 2.62$$

Regula-Falsi Method

Let $f(x)$ is continuous function. x_0, x_1 are initial guess values such that $f(x_0)$ and $f(x_1)$ having opposite signs i.e. $f(x_0)$

$$f(x_1) < 0 \text{ (say } f(x_0) < 0 \text{ and } f(x_1) > 0 \text{)}.$$

Regula-Falsi iteration formula for finding roots of $f(x)=0$ is

$$x_{n+1} = \frac{f_n x_{n-1} - f_{n-1} x_n}{f_n - f_{n-1}}$$

In particular for $n = 1$

$$x_2 = \frac{f_1 x_0 - f_0 x_1}{f_1 - f_0}$$

Case 1: If $(x_2) = 0$, then $x_2 \rightarrow$ root, stop the process

Case 2: If $f(x_2) < 0$ then compute x_3 by replacing x_0 by (x_2) and x_0 by f_2



$$x_3 = \frac{f_1 x_2 - f_2 x_1}{f_1 - f_2}$$

Case 3: If $f(x_1) > 0$ compute x_3 by replacing x_1 by x_2 and f_1 by f_2

$$x_3 = \frac{f_2 x_0 - f_0 x_2}{f_2 - f_0}$$

Continue the above process until desired accuracy of root is found. Like bisection method this is also 100% reliable. i.e. root will always be found. Both bisection and Regula-falsi method have linear convergence.

Solved Examples

Example: Find x_2 and x_3 using Regula-Falsi Method. $f(x) = x^3 + x - 1 = 0$, $x_0 = 0.5$, $x_1 = 1$

Solution: $f_0 = f(0.5) = -0.375 < 0$

$f_1 = f(1) = 1 > 0$

Then, x_2

$$= \frac{f_1 x_0 - f_0 x_1}{f_1 - f_0} = \frac{1 \times (0.5) - (-0.375)(1)}{1 - (-0.375)} = 0.636$$

$$f_2 = f(x_2) = f(0.64) = -0.0979 < 0$$

Then, the root will lie in $(0.64, 1)$. Next value x_3 can be computed as,

$$x_3 = \frac{f_1 x_2 - f_2 x_1}{f_1 - f_2} = \frac{1 \times 0.64 - (-0.0979)(1)}{1 - (-0.0979)}$$

$$x_3 = 0.672$$

Secant Method

Secant method is similar to Regula-Falsi except that in secant method initial values x_0 , x_1 need not satisfy the condition $f(x_0) f(x_1) < 0$ i.e. These two need not have opposite signs. Secant method does not provide a guarantee for existence of root in the interval $[x_0, x_1]$. So it is unreliable.

Secant method iteration formula for finding roots of the equation of $f(x)=0$, is x

$$x_n = \frac{f_n x_{n-1} - f_{n-1} x_n}{f_n - f_{n-1}}$$

Similar to Regula-Falsi method the formula for calculating x_2 is,

$$x_2 = \frac{f_1 x_0 - f_0 x_1}{f_1 - f_0}$$

In the secant method to compute x_3 replace x_0 by x_1 and x_1 by x_2 . Thus, x_3 can be calculated as,

$$x_3 = \frac{f_2 x_1 - f_1 x_2}{f_2 - f_1}$$

Solved Examples

Example: Find x_2 and x_3 using the secant

$f(x) = x^3 - 2x - 5 = 0$, $x_0 = 2$, $x_1 = 3$?

Solution: $f_0 = f(2) = -1$

$f_1 = f(x_1) = f(3) = 16$

$$x_2 = \frac{f_1 x_0 - f_0 x_1}{f_1 - f_0} = \frac{16 \times 2 + 1 \times 3}{16 + 1} = 2.058$$

$f_2 = f(x_1) = f(2.058) = 0.3907$

$$x_3 = \frac{f_2 x_1 - f_1 x_2}{f_2 - f_1} = \frac{-0.3907 \times 3 - 16 \times 2.058}{-0.3907 - 16} = 2.0804$$

Newton Raphson Method

This method gives the better result as compared to previous two methods. Let x_0 be the initial guess for the root of $f(x)=0$ and let $x_1 = x_0 + h$ be the correct root such that $f(x_1)=0$.

By Taylor's Series we obtain,

$$f(x) = f(x_0) + hf'(x_0) + f''(x_0) + \dots = 0$$

Neglecting second order and higher order derivatives.

$$\text{Then, } x_1 = x_0 - \frac{f'(x_0)}{f(x_0)}$$

Thus, Newton-Raphson formula for finding root of the equation $f(x) = 0$ is

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}$$

Newton-Raphson method has a second-order or quadratic convergence. Geometrically, in Newton-Raphson method a tangent to the curve $y = f(x)$ is drawn at first root and the intersection of the tangent with x-axis is taken as the second root and same procedure continues till there is a small difference between successive roots.



Example: If $x_{n+1} = \frac{x^n}{2} + \frac{9}{8x_n}$ and $x_0 = 0.5$ then N-R iteration formula will converge to

Solution: When the method converges, successive iterations will yield identical results i.e.

$$x_{n+1} = x_n = x$$

$$x_{n+1} = \frac{x_n}{2} + \frac{9}{8x_n}$$

$$x = \frac{x}{2} + \frac{9}{8x} \Rightarrow x^2 = \frac{9}{4} \Rightarrow x = \pm \frac{3}{2}$$

$$\therefore x = +1.5, x = -1.5$$

Since $x_0 = 0.5$, $x = 1.5$ as the method converges to the root nearest to the initial guess.

Example: Find x_1 & x_2 using the N-R formula for reciprocal of a , where $a = 7$, $x_0 = 0.2$?

Solution: Let $x = \frac{1}{a}$. This can also be expressed

as $\frac{1}{x} = a$ because for $x = \frac{1}{a} = 0$, $f''(x)$ doesn't exist.

$$f(x) = \frac{1}{x} - a = 0$$

$$f'(x) = -\frac{1}{x^2}$$

$$x_{n+1} = x_n - \frac{\left(\frac{1}{x_n} - a\right)}{\left(-\frac{1}{x_n^2}\right)} = x_n + x_n^2 \left(\frac{1-a}{x_n}\right) = 2x_n - ax_n^2$$

$$x_{n+1} = 2x_n - 1x_n^2$$

$$n = 0, x_1 = 2x_0 - ax_0^2 = 2 \times 0.2 - 7(0.2)^2 = 0.12$$

$$n = 1, x_2 = 2x_1 - ax_1^2 = 2 \times 0.12 - 7(0.12)^2 = 0.1392$$

Note: NR applicable for a function $f(x)$ only when $f''(x) \neq 0$.

Rate of Convergence

The fastness of convergence to the root is called rate of convergence.

Assume $x = 2$ is the exact root of $f(x) = 0$. The various results of iterations by different hypothetical methods have been given in the table below,

Iteration	Method 2	Method 3	Method 1
1	3	6	6
2	5	4	5
3	7	2.01	4
4	10		3
5	12		2.01

Table 6.2

In the above table rate of convergence of method 2 is higher than method 3 as it converges to root in lesser number of iterations. In method 1 when iterations are increasing it is moving away from the root. So method 1 is said to be not converging to the root.

Order of Convergence

A method is said to be convergence of order 'p' if $\epsilon_{n+1} = K \epsilon_n^p$ where K is constant.

Suppose if $f(x) = 0$ and $x = 2$ is exact root of $f(x) = 0$.

Method 1:

$$\left\{ \begin{array}{l} x_n = 2.004 ; \epsilon_n = -0.004 \\ x_{n+1} = 2.002 ; \epsilon_{n+1} = -0.002 \end{array} \right\} \epsilon_{n+1} = \frac{1}{2} \epsilon_n \dots\dots\dots (1)$$

Method 2:

$$\left\{ \begin{array}{l} x_n = 2.004 ; \epsilon_n = -0.004 \\ x_{n+1} = 2.000016 ; \epsilon_{n+1} = -0.000016 \end{array} \right\}$$

$$\epsilon_{n+1} = k \epsilon_n^2 \dots\dots\dots (2)$$

Note:

- N-R method is better than the remaining methods but it is applicable only for the curves which are having large slope values that is where the graph crosses the x-axis the required root otherwise apply any of the remaining 3 methods.
- Secant method is better than Regula Falsi and bisection. But in the secant method, there is a possibility that iteration formula may be invalid.

Suppose $f(x) = x^2$

$$x_0 = -1 \rightarrow f_0(-1) = (-1)^2 = 1$$

$$x_0 = 1 \rightarrow f_1(1) = 1^2 = 1$$

$$x_2 = \frac{f_1 x_0 - f_0 x_1}{f_1 - f_0}$$



$\therefore f_1 - f_2 = 0$ so the above formula is invalid, so secant method is inapplicable.

Numerical Methods of Integration

The area bounded by $f(x)$ and x -axis between the limits a and b is denoted by $\int_a^b f(x) dx$

Divide the interval (a, b)

into 'n' equal subintervals where the length of each interval is h (step size).

$$\text{i.e. } [a, b] = \{a = x_0, x_1, x_2, \dots, x_n = b\}$$

where $a = x_0$

$$x_1 = x_0 + h$$

$$x_2 = x_1 + x_0 + 2h$$

:

:

$$x_n = x_0 + nh$$

$$\text{i.e. } b = a + nh$$

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

To calculate these integrals, the function $f(x)$ is approximated by a polynomial using the interpolation technique. If $f(x)$ is approximated using Newton's forward difference formula the integral becomes,

$$I = \int_a^b f(x) dx = \int_{x_0}^{x_n} f(x) dx$$

$$I = \int_{x_0}^{x_n} \left[y_0 + p\Delta y_0 + \frac{p(p-1)}{2} \Delta^2 y_0 + \dots \right] dx$$

$$\Delta y_i = y_{i+1} - y_i$$

$$\Delta^2 y_i = \Delta y_{i+1} - \Delta y_i = y_{i+2} - 2y_{i+1} + y_i$$

$$\text{Similarly, } \Delta^n y_i = \Delta^{n-1} y_{i+1} - \Delta^{n-1} y_i$$

Each of the terms above is called as forward difference.

$$y_i = f(x_i)$$

where $i \in [1, n]$

if $x = x_0 + ph$ then $dx = hdp$ then above integral comes out to be,

$$I = nh \left[y_0 + \frac{n}{2} \Delta y_0 + \frac{n(n-3)}{12} \Delta^2 y_0 + \frac{n(n-2)^2}{24} \Delta^3 y_0 + \dots \right]$$

Trapezoidal Rule

By this rule, the area under the curve is approximated by a trapezoid or multiple trapezoids. Each trapezoid has a width 'h' and the two parallel sides have length y_{i-1} & y_i .

This can also be understood in terms that the curve between two successive points will be approximated by a straight line or linear approximation.

Thus, if we put $n=1$, the forward differences higher than first will go to zero.

$$I = \int_{x_0}^{x_1} y dx = h \left[y_0 + \frac{1}{2} \Delta y_0 \right] = h \left[y_0 + \frac{1}{2} (y_1 - y_0) \right] \\ = \frac{h}{2} [y_0 + y_1]$$

$$\text{Similarly, } I = \int_x^{x_{i+1}} y dx = h \left[y_i + \frac{1}{2} \Delta y_i \right] = \frac{h}{2} [y_i + y_{i+1}]$$

Adding all such integrals we get,

$$\int_a^b f(x) dx = \frac{h}{2} [(y_0 + y_n) + 2(y_1 + y_2 + \dots + y_{n-1})]$$

Simpson's 1/3 Rule or Simpson's Rule (N divisible by 2)

In this rule, the curve is approximated by $n/2$ arcs of second order polynomials. So, we consider three points at a time to construct a second order polynomial.

This can be obtained by substituting $n=2$ in the general formula,

$$I = \int_{x_0}^{x_2} y dx = 2h \left[y_0 + \Delta y_0 \frac{1}{6} \Delta^2 y_0 \right] \\ = \frac{h}{3} [6y_0 + 6(y_1 - y_0) + (y_2 - 2y_1 + y_0)]$$

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

All forward difference higher than the second are zero.

Generally,

$$I = \int_{x_{i-1}}^{x_{i+1}} y dx = \frac{h}{3} [6y_{i-1} + 6(y_i - y_{i-1}) + (y_{i+1} - 2y_{i-1})] \\ = \frac{h}{3} [y_{i-1} + 4y_i + y_{i+1}]$$



Summing $a|h|$ such terms we get,

$$\int_a^b f(x) dx = 3 \left[(y_0 + y_n) + 2(y_2 + y_4 + \dots + y_{n-2}) + 4(y_1 + y_3 + y_5 + \dots + y_{n-1}) \right]$$

The only limitation with this rule is that we need to divide the interval into even number of subintervals.

Simpson's 3/8 Rule (N divisible by 3)

This rule is obtained by putting $n=3$ in the general formula. Though this rule is not so accurate as Simpson's 1/3 rule.

$$\int_a^b f(x) dx = \frac{3h}{8} \left[(y_0 + y_n) + 2(y_3 + y_6 + \dots + y_{n-3}) + 3(y_1 + y_2 + y_4 + y_5 + \dots + y_{n-1}) \right]$$

Solved Examples

Example: The table below gives values of a function $F(x)$ obtained for values of x at intervals of 0.25. Evaluate

$$\int_0^1 f(x) dx \text{ using Simpson's Rule.}$$

x	0	0.25	0.5	0.75	1
$f(x)$	1	0.9412	0.8	0.64	0.5

Table 6.3

The value of integral between the limits 0 and 1 using Simpson's Rule is

Solution: By default Simpson's $\frac{1}{3}$ rule is called Simpson's Rule.

Simpson's $\frac{1}{3}$ Rule

$$\begin{aligned} &= \frac{h}{3} [(y_0 + y_4) + 2y_2 + 4(y_1 + y_3)] \\ &= \frac{0.25}{3} [(1 + 0.5) + 2(0.8) + 4(0.9412 + 0.64)] \\ &= 0.7854 \end{aligned}$$

Example: The integral $\int_1^3 \frac{1}{x} dx$ when evaluated using Simpson's Rule on two equal intervals with length of each interval is 1, equals

Solution: Evaluating all the subintervals and values of function at the sub-interval boundaries,

x	$\frac{1}{x}$
$x_0 = 1$	$1 \ y_0$
$x_1 = 2$	$1/2 \ y_1$
$x_2 = 3$	$1/3 \ y_2$

Table 6.4

$$\begin{aligned} \text{simpson } \frac{1}{3} \text{ Rule} &= \frac{1}{3} [(y_0 + y_2) + 4y_1] \\ &= \frac{1}{3} \left[1 + \frac{1}{3} + \frac{1}{9} \right] = \frac{10}{9} \end{aligned}$$

Example: The integral $\int_0^{2\pi} \sin x \, dx$

is evaluated using Trapezoidal Rule on 8 equal intervals with '5' significant digits.

$$\text{Solution: } h = \frac{b-a}{n} = \frac{2\pi - 0}{8} = \frac{\pi}{4}$$

$$T - \text{Rule} = \frac{h}{2}$$

$$\begin{aligned} &[(y_0 + y_8) + 2(y_1 + y_2 + y_3 + y_4 + y_5 + y_6 + y_7)] \\ &= \frac{\pi}{8} [0 + 0 + 2(0.7071 + 1 + 0.7071 - 1 - 0.7071)] = 0 \end{aligned}$$

5 significant digits are required = 0.00000

x	$\sin x$
x_0	y_0
$x_1 = \frac{\pi}{4}$	$y_1 = 0.70710$
$x_2 = \frac{\pi}{2}$	$y_2 = 1$
$x_3 = \frac{3\pi}{4}$	$y_3 = 0.70710$
$x_4 = \pi$	$y_4 = 0$
$x_5 = \frac{5\pi}{4}$	$y_5 = -0.70710$
$x_6 = \frac{6\pi}{4}$	$y_6 = -1$
$x_7 = \frac{7\pi}{4}$	$y_7 = -0.70710$
$x_8 = \frac{8\pi}{4}$	$y_8 = 0$

Table 6.5



Truncation Error

Let $f(x)$ is a function defined in the interval $[x_0, x]$ where $(x - x_0) = h$.

Expand $f(x)$ about x_0 using Taylor series expansion.

$$f(x) = f(x_0) + (x - x_0)f'(x_0) + (x - x_0)^2 f''(x_0) + \dots + \frac{(x - x_0)^n}{n!} f^{(n)}(x_n) + R$$

$$\text{where } R = \frac{(x - x_0)^{n+1}}{(n+1)!} f^{(n+1)}(\phi)$$

If we consider only terms upto 'n' then we neglect R. Thus, R will be called as Truncation Error.

Truncation error bound denoted by |R| and

$$|R| \leq \left| \max \left(\frac{(x - x_0)^{n+1}}{(n+1)!} f^{(n+1)}(\phi) \right) \right|_{(x_0, x)}$$

Here, $\phi \in [x_0, x]$

Solved Examples

Example: If we approximate $e^x = 1 + x + \frac{x^2}{2!}$

then find (i) T.E. (ii) |T.E| in $[2, 3]$?

Solution: The Taylor's Series for e^x

$$e^x = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \frac{x^4}{4!} + \dots$$

$$f(x) = f(x_0) + (x - x_0)f'(x_0) + (x - x_0)^2 f''(x_0) + \dots$$

Comparing $f(x) = e^x$ and $x_0 = 0$

$$f(x_0) = e^0 = 1$$

$$f'(x_0) = e^0 = 1$$

The truncation error is given by,

$$R = \frac{(x - x_0)^{n+1}}{(n+1)!} f^{(n+1)}(\phi), \quad x_0 \leq \phi \leq x$$

$$R = \frac{(x - 0)^3}{3!} f^{(3)}(\phi)$$

$$|TE| = R = \frac{x^3}{3!} 2^\phi$$

$$x_0 \leq \phi \leq x$$

$$\text{ii) } |TE| \leq \left| \max \left(\frac{x^3}{3!} e^\phi \right) \right|_{[2,3]} \leq \frac{3^5}{e^3}$$

$$|TE| \leq \frac{27}{6} 3^3$$

Truncation Error in Numerical Integration

Trapezoidal Rule

$$T_{E(\max)} = -\frac{h^3}{12} N f''(x) = \frac{(b-a)}{12} h^2 f''(x)$$

Where, $x \in [x_0, x_n]$ and $h = \frac{b-a}{N}$ is the step size

The maximum value of Truncation Error can be,

$$|T_E|_{(\max)} = \frac{h^2}{12} (b-a) \times \max |f''(x)|$$

Simpson's 1/3 Rule

The Truncation Error for simple Simpson's Rule with 3 points is given by,

$$T_E = \frac{n}{90} f^{(iv)}(x)$$

If there are N intervals then,

$$T_{E(\max)} = \frac{h^5}{90} N f^{(iv)}(x)$$

$$\text{Where, } N = \frac{b-a}{h}$$

The maximum value of Truncation Error can

$$\text{be, } T_E = \frac{h^4}{180} (b-a) \times \max |f^{(iv)}(x)|$$

Simpson's 3/8 Rule

The Truncation Error for simple Simpson's

$$3/8 \text{ Rule is given by, } T_E = \frac{h^4}{80} (b-a) f^{(iv)}(x)$$

Where, $x \in [x_0, x_n]$ and $h = \frac{b-a}{N}$ is the step size.

The maximum value of Truncation Error can be,



$$|T_E|_{(max)} = \frac{h^4}{80}(b-1) \times \max |f^{(iv)}(x)|$$

Important Points

- Trapezoidal Rule evaluates the polynomial with exact results and they are having upto degree 1 (0 or 1).
- In Simpsons rule we truncated 4th order derivative. It evaluates the polynomials with exact results if they are having degree upto 3 (0, 1, 2 or 3).
- T Rules is applicable on any number of intervals.
- Simpson's 1/3 rule is applicable only if number of intervals are multiples of 2. (n=2 (or) 4 (or) 6).
- Simpson's 3/8 rule is applicable if the number of intervals are multiples of 3. (n = 3 (or) 6 (or) 9)
- Error order in Trapezoidal Rule is order of h^3
- Error order in Simpson 1/3 Rule is order of h^5
- Error order in Simpson 3/8 Rule is order of h^5

Solved Examples

Example: Minimum number of equivalent subintervals needed to approximate $\int_1^2 xe^x dx$ to an accuracy at least $\frac{1}{3} \times 10^{-6}$

Solution: $f(x) = e^x$

$$a = 1, b = 2$$

$$f'(x) = e^x + xe^x$$

$f''(x) = 2e^x + xe^x$ which is an increasing function.

$$\max |f''(x)|_{[1,2]} = 4e^2 (x = 2)$$

$$\text{Since, Accuracy} \geq \frac{1}{3} \times 10^{-6}$$

$$\text{Thus, } |T_E| \leq \frac{1}{3} \times 10^{-6}$$

For Trapezoidal Rule,

$$\left| \frac{b-1}{12} \times h^2 \times \max f''(x) \right| \leq \frac{1}{3} \times 10^{-6}$$

$$\frac{2-1}{12} \times h^2 \times 4e^2 \leq \frac{1}{3} \times 10^{-6}$$

$$h^2 \times e^2 \leq 10^{-6}$$

$$h = \frac{b-a}{n} = \frac{2-1}{n} = \frac{1}{n}$$

$$\frac{1}{n^2} \times e^2 \leq 10^{-6}$$

$$e^2 \times 10^6 \leq n^2$$

$$n \geq 1000e$$

Example: The minimum number of subintervals needed to approximate

$\frac{8}{45} \times 10^{-8}$ using Simpson's Rule is?

Solution: $f(x) = e^{2x}$

$$a = 0, b = 2$$

Successive derivatives of the function are,

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

$$f''(x) = 4e^{2x}$$

$$f'''(x) = 8e^{2x}$$

$$f^{(iv)}(x) = 16e^{2x}$$

$\max |f^{(iv)}(x)|_{[0,2]} = 16e^4$ as it is an increasing function so maxima occur at the end point of interval.

$$\text{Since, Accuracy} \geq \frac{8}{45} \times 10^{-8}$$

$$|T_E| \geq \frac{8}{45} \times 10^{-8}$$

For Simpson's 1/3 rule

$$\left| \frac{(b-1)}{180} h^4 \times f^{(iv)}(x) \right| \leq \frac{8}{45} \times 10^{-8}$$

$$\frac{2}{180} \times h^4 \times 16e^4 \leq \frac{8}{45} \times 10^{-8}$$

$$h^4 e^4 \leq 1^{-8}$$

$$n = \frac{b-a}{h} = \frac{2}{h}$$

$$\left(\frac{2}{n} \right)^4 e^4 \leq 1^{-8}$$

$$\frac{2^4}{n^4} e^4 \leq 10^{-8}$$

$$n^4 \geq 2^4 \times e^4 \times 10^8$$

$$n \geq 2 \times 2 \times 10^2$$

$$n \geq 200e$$



Numerical Solution of Differential

Equations

Analytically, only a limited set of differential equations can be solved. The most common type of differential equations occurring practically cannot be solved by analytical methods. They have to be solved numerically. The differential equation can be represented as,

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

The condition $y(x_0) = y_0$ is called as Initial Conditions and this problem is called as Initial Value Problem. The problems where values are specified at more than one point are called as Boundary Value Problems.

Euler's Method

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

$$y_{i+1} = y_i + hf(x_i, y_i)$$

In particular for $i = 0, y_1 = y_0 + hf(x_0, y_0)$

Here, h represents the step size for the numerical integration.

In Euler's Method, we approximate the curve of solution by the tangent in each interval and thus for the method to be accurate h must be small. Else, the tangent may deviate considerably from the curve.

Solved Examples

Example: $\frac{dy}{dx} = x + y, y(0) = 1, h = 0.1$ find $y(0.2)$ using Euler's method?

Solution: $\frac{dy}{dx} = x + y, y(0) = y', x_0 = 0, y_0 = 1$

x	y	Comment
$x_0 = 0$	$y_0 = 1$	Initial condition
$x_1 = 0.1$	$y_0 = 1.1$	$y_1 = y_0 + hf(x_0, y_0)$ $= 1 + 0.1(x_0 + y_0)$ $= 1 + 0.1(0 + 1) = 1.1$
$x_2 = 0.2$	$y_2 = 1.22$	$y_1 = y_1 + hf(x_1, y_1)$ $= 1.1 + 0.1(x_1 + y_1)$ $= 1 + 0.1(0.1 + 1.1) = 1.22$

Example: $\frac{dy}{dx} - y = x, y(0) = 0, h = 0.1$. Find $y(0.3)$ using Euler's method?

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

$$y_0 = 0, x_0 = 0, h = 0.1$$

$$y_1 = y_0 + hf(x_0, y_0) = 0 + 0.1(x_0 + y_0) = 0$$

$$y_2 = y_1 + hf(x_1, y_1) = 0 + 0.1(0.1 + 0) = 0.01$$

$$y_3 = y_2 + hf(x_2, y_2) = 0.01 + 0.1(0.2 + 0.01) = 0.031$$

Backward Euler's Method (Implicit Euler's Method)

$$y_{i+1} = y_i + hf(x_{i+1}, y_{i+1})$$

y_{i+1} appears on LHS as well as RHS

Any Numerical method where y_{i+1} appears on LHS and RHS is called an implicit method. In Euler's Method y_{i+1} only appears on LHS so it is called as explicit method.

Solved Examples

Example: $\frac{dy}{dx} = x + y, y(x_0) = y_0, y(0) = 1, h = 0.1$, find $y(0.2)$ using Implicit Euler's Method.

Solution: $\frac{dy}{dx} = f(x, y) = x + y, x_0 = 0, y_0$

$$y_{i+1} = y_i + hf(x_{i+1}, y_{i+1})$$

$$y_{i+1} = y_i + h(x_{i+1} + y_{i+1})$$

$$(1 - h)y_{i+1} = y_i + hx_{i+1}$$

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

x	y	Comment
$x_0 = 0$	$y_0 = 1$	Initial condition
$x_1 = 0.1$	$y_0 = 1.1$	$y_1 = \frac{y_0 + hx_1}{(1 - h)}$ $= \frac{1 + 0.1[0.1]}{1 - 0.1} = 1.12$



$x_2 = 0.2$	$y_2 = 1.22$	$y_1 = \frac{y_1 + hx_2}{(1-h)}$ $= \frac{1.12 + 0.1[0.2]}{1-0.1} = 1.26$
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Table 6.6

Example: $\frac{dy}{dx} = 0.25y^2, y(0) = 1, h = 1$. Find $y(1)$ using implicit Euler's Method?

Solution: $y_{i+1} = y_i + hf(x_{i+1}, y_{i+1})$

$$y_0 = 1, y_1 = y_0 + h(0.25)y_1^2$$

$$0.25y_1^2 - y_1 + 1 = 0$$

$$y_1 = 2$$

Runge-Kutta Method

Runge-Kutta Method is most commonly used to find numerical solution of differential equations and it has different orders. The accuracy of approximation increases as the order of Runge-Kutta Method.

Second Order Method or Modified Euler method

$$y = y + \frac{1}{2}(k_1 + k_2)$$

$$\text{Where, } k_1 = hf(x_i, y_i)$$

$$k_2 = hf(x_i + h, y_i + k_1)$$

Third Order Method

$$y_{i+1} = y_i + \frac{1}{6}(k_1 + 4k_2 + k_3)$$

$$\text{Where, } k_1 = hf(x_i, y_i)$$

$$k_2 = hf\left(x_i + \frac{h}{2}, y_i + \frac{k_1}{2}\right)$$

$$k_3 = hf(x_i + h, y_i + k_2)$$

Fourth Order Method

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

$$\text{Where } k_1 = hf(x_i, y_i)$$

$$k_2 = hf\left(x_i + \frac{h}{2}, y_i + \frac{k_1}{2}\right)$$

$$k_3 = hf\left(x_i + \frac{h}{2}, y_i + \frac{2}{2}\right)$$

$$k_4 = hf(x_i + h, y_i + k_3)$$

Solved Examples

Example: $\frac{dy}{dx} = x - y, y(0) = 0, h = 0.2$ dx
Find $y(0.2)$ using second order Runge Kutta?

Solution:

$$\frac{dy}{dx} = f(x, y) = x - y, x_0 = 0, y_0 = 0, h = 0.2$$

$$\text{Second order Formula is } y_0 = y_1 + \frac{1}{2}(k_1 + k_2)$$

$$\text{Where } k_1 = hf(x_0, y_0) = 0.2(x_0 - y_0) = 0$$

$$k_2 = hf(x_0 + h, y_0 + k_1) = 0.2((x_0 + h) - (y_0 + k_1))$$

$$= 0.2((0 + 0.2) - (0 + 0)) = 0.04$$

$$y_1 = 0 + \frac{1}{2}(0 + 0.04) = 0.02$$

Example: $\frac{dy}{dx} = x + y, y(0) = 1, h = 0.2$

find $y(0.2)$ using

(a) Fourth Order RK

(b) Third order RK

Solution: Third Order Runge-Kutta

$$k_1 = hf(x_0, y_0) = 0.2 \times (x_0 + y_0) = 0.2 \times (0 + 1)$$

$$= 0.2$$

$$k_2 = hf\left(x_0 + \frac{h}{2}, y_0 + \frac{k_1}{2}\right)$$

$$= 0.2 \times \left(0 + \frac{0.2}{2} + 1 + \frac{0.2}{2}\right) = 0.24$$

$$k_3 = hf(x_0 + h, y_0 + k_2) = 0.2 \times (0 + 0.2 + 1 + 0.24)$$

$$= 0.288$$

$$y_1 = y_0 + \frac{1}{6}(k_1 + 4k_2 + k_3)$$

$$= 1 + \frac{1}{6}(0.2 + 4 \times 0.24 + 0.88)$$

$$y_1 = 1.1151$$

Fourth Order Runge-Kutta

$$k_1 = hf(x_0, y_0) = 0.2(x_0 + y_0) = 0.2 \times (0 + 1)$$

$$= 0.2$$

$$k_2 = hf\left(x_0 + \frac{h}{2}, y_0 + \frac{k_1}{2}\right)$$

$$= 0.2 \times \left(0 + \frac{0.2}{2} + 1 + \frac{0.2}{2}\right) = 0.24$$

$$k_3 = hf\left(x_0 + \frac{h}{2}, y_0 + \frac{k_2}{2}\right)$$



$$= 0.2 \times \left(0 + \frac{0.2}{2} + 1 + \frac{0.24}{2} \right) = 0.244$$

$$k_4 = hf(x_0 + h, k_3)$$

$$= 0.2 \times (0 + 0.2 + 1 + 0.244) = 0.2888$$

$$y_1 = 1 + \frac{1}{6} (0.2 + 2 \times 0.24 + 2 \times 0.244 + 0.288)$$

$$y_1 = 1.24267$$

Stability Analysis in Euler's Method

Consider Euler's equation $y_{i+1} = y_i + hf(x_i, y_i)$
 Convert the equation into the form $y_{i+1} = Ey_i + hk$ Where K is constant or it contains ' x_i ' terms. The above equation is said to be stable if $E \leq 1$

Solved Examples

Example: $\frac{dx}{dt} = \frac{1-x}{T}$ with step size $\Delta T > 0$ is evaluated using Euler's method. What is the maximum permissible value of ΔT to ensure the stability in the solution?

Solution: $\frac{dx}{dt} = \frac{1-x}{T}$ The given differential equation is,

This can be reframed as,

$$\frac{dy}{dx} = f(x, y) = \frac{1-y}{T}$$

By Euler's Method we have,

$$y_{i+1} = y_i + hf(x_i, y_i)$$

$$y_{i+1} = \left(\frac{1-y_i}{T} \right)$$

$$y_{i+1} = \left(1 - \frac{h}{T} \right) y_i + \frac{h}{T}$$

$$\text{Where } E = 1 - \frac{h}{T}, k = \frac{1}{T}$$

System is stable if $|E| \leq 1$

$$\left| 1 - \frac{h}{T} \right| \leq 1$$

$$\left| 1 - \frac{\Delta T}{T} \right| \leq 1$$

$$-1 \leq 1 - \frac{\Delta T}{T} \leq 1$$

$$-2 \leq -\frac{\Delta T}{T} \leq 1$$

$$0 \leq \Delta T \leq 2$$

Hence, the maximum permissible value of ΔT is $2T$.

Note: The order of error by different methods in Numerical Integration is given below,

Method	Error Order
Euler's (First Order R.K)	$O(h^2)$
2 nd Order R.K	$O(h^3)$
3 rd Order R.K	$O(h^4)$
4 th Order R.K	$O(h^5)$

Table 6.7

Chapter Summary

Numerical solution of algebraic equations

- Descartes Rule of sign**

An equation $f(x) = 0$ cannot have more positive roots than the number of sign changes in (x) & cannot have more negative roots than the number of sign changes in $f(-x)$

- Bisection Method**

If a function $f(x)$ is continuous between a & $f(a)$ & $f(b)$ are of opposite sign, then thereat least one of $f(x)$ between a & b

Since root lies between a & b , we assume

$$\text{root } x_0 = \frac{(a+b)}{2}$$

If $f(x_0) = 0$; x_0 is the root

Else, if $f(x_0)$ has same sign as $f(a)$, then roots lies between x_0 & b and we assume

$$x_1 = \frac{x_0 + b}{2} \text{ and follow same procedure if } f(x_0)$$

has same sign as $f(b)$, then

root lies between a & x_0 & we assume $x_1 = \frac{a + x_0}{2}$ & follow same procedure.



We keep on doing is, till is close zero.

No. of step required to achieve and accuracy ϵ

$$n \geq \frac{\log_e \left(\frac{|b-a|}{\epsilon} \right)}{\log_e 2}$$

- **Regula-falsi Method**

This method is similar to bisection method, as we assume two value x_0 & x_1 Such that $f(x_0)f(x_1) < 0$

$$x_2 = \frac{f(x_1) - x_0 - f(x_0) - x_1}{f(x_1) - f(x_0)}$$

If $f(x_2) = 0$ then x_2 is the root, stop the process

If $f(x_2) > 0$ then

$$x_3 = \frac{f(x_2)x_0 - f(x_0)x_2}{f(x_2) - f(x_0)}$$

If $f(x_2) < 0$ then

$$x_3 = \frac{f(x_1)x_2 - f(x_2)x_1}{f(x_1) - f(x_2)}$$

- **Regula-falsi Method**

IID. secant method, we remove the condition that $f(x_0)f(4) < 0$ and it doesn't provide the guarantee for existence of the root **m** the given interval, So it is called in reliable method.

and to compute X_3 replace every variable by its variable **m** -12

$$x_3 = \frac{f(x_2) \cdot x_1 - f(x_1) \cdot x_2}{f(x_2) - f(x_1)}$$

Continue the above process till required not not found

- **Newton-Raphson Method**

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}$$

Note: Since R iteration method is qu this formufa must exist $f(x)$

Order of convergence

- Bisection Linear
- Regula Falsi Linear

Secant

Newton. Raphson.=

Superliners

Quadratic

- **Numerical Intergration Trapezoidal Rule**

$\int_a^b f(x) dx$, can be calculated as

Divide interval (a, n) into n sub-intervals

such that width od each interval

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

we have $(n+1)$ point at edged of each intervals

$$(x_0, x_1, x_2, \dots, x_n)$$

$$y_0 = f(x_0) = y_1 = f(x_1), \dots, y_n = f(x_n)$$

$$\int_a^b f(x) dx = \frac{h}{2} [y_0 + 2(y_1 + y_2 + \dots + y_{n-1}) + y_n]$$

- **Simpson's 1/3rd Rule**

Here the number of intervals should be even

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

$$\int_a^b f(x) dx = \frac{h}{3} [y_0 + 4(y_1 + y_3 + y_5 + \dots + y_{n-1}) + 2(y_2 + y_4 + \dots + y_{n-2}) + y_n]$$

Simpson's $\frac{3}{8}$ th Rule

Here the number of intervals should be even

$$\int_a^b f(x) dx = \frac{3h}{8} [y_0 + 3(y_1 + y_2 + y_4 + y_5 + \dots + y_{n-1}) + 2(y_3 + y_6 + y_9 + \dots + y_{n-3}) + y_n]$$

- **Simpson's 1/3rd Rule**

$$\text{Trapezoidal Rule : } |T_e|_{\text{bound}} = \frac{(b-a)}{12} h^2 \max$$

$|f''(\epsilon)|$ and order of error = 2

$$\text{Simpson's } \frac{1}{3} \text{ Rule : } |T_e|_{\text{bound}} = \frac{(b-a)}{180} h^4 \max$$

$|f^{(iv)}(\epsilon)|$ and order of error = 4

$$\text{Simpson's } \frac{3}{8} \text{ Rule : } |T_e|_{\text{bound}} = \frac{3(b-a)}{n180} h^4 \max$$

$|f^{(iv)}(\epsilon)|$ and order of error = 5

Where $x_0 \leq \epsilon \leq x_n$



Note: If truncation error occurs at nth order derivation then given exact result while integrating the polynomial up to degree (n-)

Numerical solution of Differential equation

Euler's Method

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

To solve differential equation by numerical method, we define a step size h

We can calculate of y at $(x_0+h, x_0+2h, \dots, x_0+nh)$ & not any intermediate points

$$y_{i+1} = y_i + hf(x_i, y_i)$$

$$y_i = y(x_i); y_{i+1} = y(x_{i+1}); x_{i+1} = x_i + h$$

Modified Euler's Method (Heun's method)

$$y_i = y_0 + \frac{h}{2} [f(x_0, y_0) + f(x_0 + h, y_0 + h)]$$

Runge-Kutta Method

$$y_i = y_0 + k$$

$$k = \frac{1}{6} (k_1 + 2k_2 + k_4)$$

$$k_1 = hf(x_0, y_0)$$

$$k_2 = hf\left(x_0 + \frac{h}{2}, y_0 + \frac{k_1}{2}\right)$$

$$k_3 = hf\left(x_0 + \frac{h}{2}, y_0 + \frac{k_2}{2}\right)$$

$$k_4 = hf(x_0 + h, y_0 + k_3)$$

Similar method for other iterations