

matrix inversion.

Another way to obtain the solⁿ of an equation of type

$$Ax = b \quad \dots \dots \dots \textcircled{1}$$

is by using matrix algebra.

Multiplying eqⁿ $\textcircled{1}$ by inverse of A gives

$$A^{-1}Ax = A^{-1}b \quad \dots \dots \dots \textcircled{2}$$

Since $A^{-1}A = I$, the identity matrix, the equation $\textcircled{2}$ becomes

$$x = A^{-1}b \quad \dots \dots \dots \textcircled{3}$$

Equation $\textcircled{3}$ gives the solution for x.

Computing matrix inverse.

This is done as follows.

① Augment the coefficient matrix A with an identity matrix as shown below,

$$\left[\begin{array}{ccc|ccc} a_{11} & a_{12} & a_{13} & 1 & 0 & 0 \\ a_{21} & a_{22} & a_{23} & 0 & 1 & 0 \\ a_{31} & a_{32} & a_{33} & 0 & 0 & 1 \end{array} \right]$$

② Apply Gauss-Jordan method to the augmented matrix to reduce A to an identity matrix, the result will be

$$\left[\begin{array}{ccc|ccc} 1 & 0 & 0 & a_{11}' & a_{12}' & a_{13}' \\ 0 & 1 & 0 & a_{21}' & a_{22}' & a_{23}' \\ 0 & 0 & 1 & a_{31}' & a_{32}' & a_{33}' \end{array} \right]$$

The right hand side of the augmented matrix is the inverse of A. Now, we can obtain the solⁿ as

$$x_1 = a_{11}'b_1 + a_{12}'b_2 + a_{13}'b_3$$

$$x_2 = a_{21}'b_1 + a_{22}'b_2 + a_{23}'b_3$$

$$x_3 = a_{31}'b_1 + a_{32}'b_2 + a_{33}'b_3$$

III-conditioned system.

Proper solution depends on the condition of the system. Systems where small changes in the coefficient result in large deviations in the solution are said to be III-conditioned system. A wide range of answers can satisfy such equations. Graphically if two lines are almost parallel, then we can say the system is III-conditioned since it's hard to decide just at which point they intersect.

Mathematically, the problem of III condition is described as follows.

$$a_{11}x_1 + a_{12}x_2 = b_1$$

$$a_{21}x_1 + a_{22}x_2 = b_2$$

If two lines are almost parallel, their slopes must be nearly equal.

$$\frac{a_{11}}{a_{12}} \approx \frac{a_{21}}{a_{22}}$$

Alternatively,

$$a_{11}a_{22} - a_{12}a_{21} \approx 0$$

Note that $a_{11}a_{22} - a_{12}a_{21}$ is the determinant of the coefficient matrix A.

$$A = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix}$$

This shows that the determinant of III-conditioned system is very small or nearly equals to zero.

By solve the following equations:

$$2x_1 + x_2 = 25$$

$$2.001x_1 + x_2 = 25.01$$

and thereby discuss the effect of ill condition.

Sol:

Given equation is

$$2x_1 + x_2 = 25$$

$$2.001x_1 + x_2 = 25.01$$

Solving those equations we get

$$x_1 = 10$$

$$x_2 = 5$$

Let us change the coefficient of x_1 in the second equation to 2.0005 we get. Now, the value of x_1 & x_2 are,

$$2x_1 + x_2 = 25$$

$$2.0005x_1 + x_2 = 25.01$$

we get,

$$x_1 = -20$$

$$x_2 = -15$$

A small change in one of the coefficient has resulted in a large change in result. This illustrates the effect of roundoff errors in ill-conditioned system.

matrix factorization.

Triangular Factorization method:

The coefficient matrix A of a system of linear equation can be factorized or decompose in two triangular matrices L and U such that,

$$A = LU \quad \dots \quad (1)$$

where,

$$L = \begin{bmatrix} l_{11} & 0 & \dots & 0 \\ l_{21} & l_{22} & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ l_{n1} & l_{n2} & \dots & l_{nn} \end{bmatrix}$$

and

$$U = \begin{bmatrix} u_{11} & u_{12} & \dots & u_{1n} \\ 0 & u_{22} & \dots & u_{2n} \\ 0 & \vdots & \ddots & \vdots \\ 0 & \vdots & \vdots & u_{nn} \end{bmatrix}$$

L is known as lower triangular & U is known as upper triangular matrix.

Once A is factorized into L and U the system of equations

$$Ax = b$$

can be expressed as

$$LUX = b$$

$$\text{or } L[UX] = b \quad \text{--- (1)}$$

let us assume that,

$$Ux = z \quad \text{--- (2)}$$

where z is an unknown vector.

Substituting eq (2) in (1) we get

$$Lz = b \quad \text{--- (3)}$$

Now we can solve the system, $Ax = b$ in two stages

(1) Solve the equation $Lz = b$ for z , by forward substitution.

(2) Solve the equation $Ux = z$ for x , using z (found in stage 1) by backward substitution.

Again to make a unique factor we assume the diagonal elements of L or U to be unity.

The decomposition with L having unit diagonal values is called Dolittle LU decomposition while the other one with U having unique unit diagonal element is called Crout LU decomposition.

Theoretical algorithm (Dolittle LU Decomposition)

- we can solve for the component of L and U given A as follows

$$A = LU$$

implies that

$$a_{ij} = l_{i1} u_{1j} + l_{i2} u_{2j} + \dots \quad \text{for } i < j$$

$$a_{ij} = l_{i1} u_{1j} + l_{i2} u_{2j} + \dots \quad \text{for } i = j$$

$$a_{ij} = l_{i1} u_{1j} + l_{i2} u_{2j} + \dots \quad \text{for } i > j$$

where,

$$u_{ij}^0 = 0 \text{ for } i > j \text{ and}$$

$$l_{ij}^0 = 0 \text{ for } i < j.$$

The Dolittle algorithm assumes that all the diagonal elements of L are unity,

$$\text{i.e. } l_{ii}^0 = 1 \text{ for } i = 1, 2, \dots, n.$$

using equation ① ② & ③ we can successively determine the elements of U and L as follows,

$$l_{ij}^0 = \frac{a_{ij}}{a_{ii}^0} - \sum_{k=1}^{i-1} l_{ik}^0 u_{kj}^0, \quad j = 1, 2, \dots, n$$

where

$$a_{ii}^0 = a_{11}, \quad u_{12}^0 = a_{12}, \quad u_{13}^0 = a_{13}$$

Similarly,

$$l_{ij}^0 = \frac{1}{u_{ii}^0} \times \left[a_{ij} - \sum_{k=1}^{j-1} l_{ik}^0 u_{kj}^0 \right] \quad j = 1, 2, \dots, n$$

where

$$l_{11}^0 = l_{22}^0 = l_{33}^0 = 1, \quad \text{and}$$

$$l_{11}^0 = \frac{a_{11}}{u_{11}^0} \quad \text{for } i = 2 \text{ to } n$$

$$\begin{array}{r} 8 \\ \times 64 \\ \hline 108 \end{array}$$

108

$$\text{or, } 107 \times \frac{1}{2} + U_{22} = 84$$

$$\text{or } U_{22} = 84 - \frac{107}{2}$$

$$\begin{aligned} \text{or } U_{22} &= \frac{108 - 107}{2} \\ &= \frac{1}{2}, \end{aligned}$$

$$\text{again, } U_{13} l_{21} + U_{23} = 20$$

$$\text{or } 36 \times \frac{1}{2} + U_{23} = 20$$

$$\text{or, } 18 + U_{23} = 20$$

$$U_{23} = 2, \quad //$$

$$\text{again } l_{31} U_{11} = 31$$

$$\text{or } l_{31} \times 50 = 31$$

$$l_{31} = \frac{31}{50}, \quad //$$

again

$$l_{31} U_{12} + l_{32} U_{22} = 66$$

$$\text{or, } \frac{31}{50} \times 107 + l_{32} \times \frac{1}{2} = 66$$

$$\text{or, } \frac{3317}{50} + \frac{l_{32}}{2} = 66$$

$$\text{or } \frac{l_{32}}{2} = 66 - \frac{3317}{50}$$

$$\text{or } \frac{l_{32}}{2} = \frac{3300 - 3317}{50}$$

114

$$\text{or } \frac{l_{32}}{2} = -\frac{17}{50}$$

$$\text{or } l_{32} = -\frac{34}{50}$$

$$= -\frac{17}{25} //$$

and,

$$l_{31}u_{13} + l_{32}u_{23} + u_{33} = 21$$

$$\text{or, } \frac{31}{50} \times 36 + \left(-\frac{17}{25} \times 2\right) + u_{33} = 21$$

$$\text{or, } \frac{1116}{50} - \frac{34}{25} + u_{33} = 21$$

$$\text{or, } u_{33} = 21 + \frac{34}{25} - \frac{1116}{50}$$

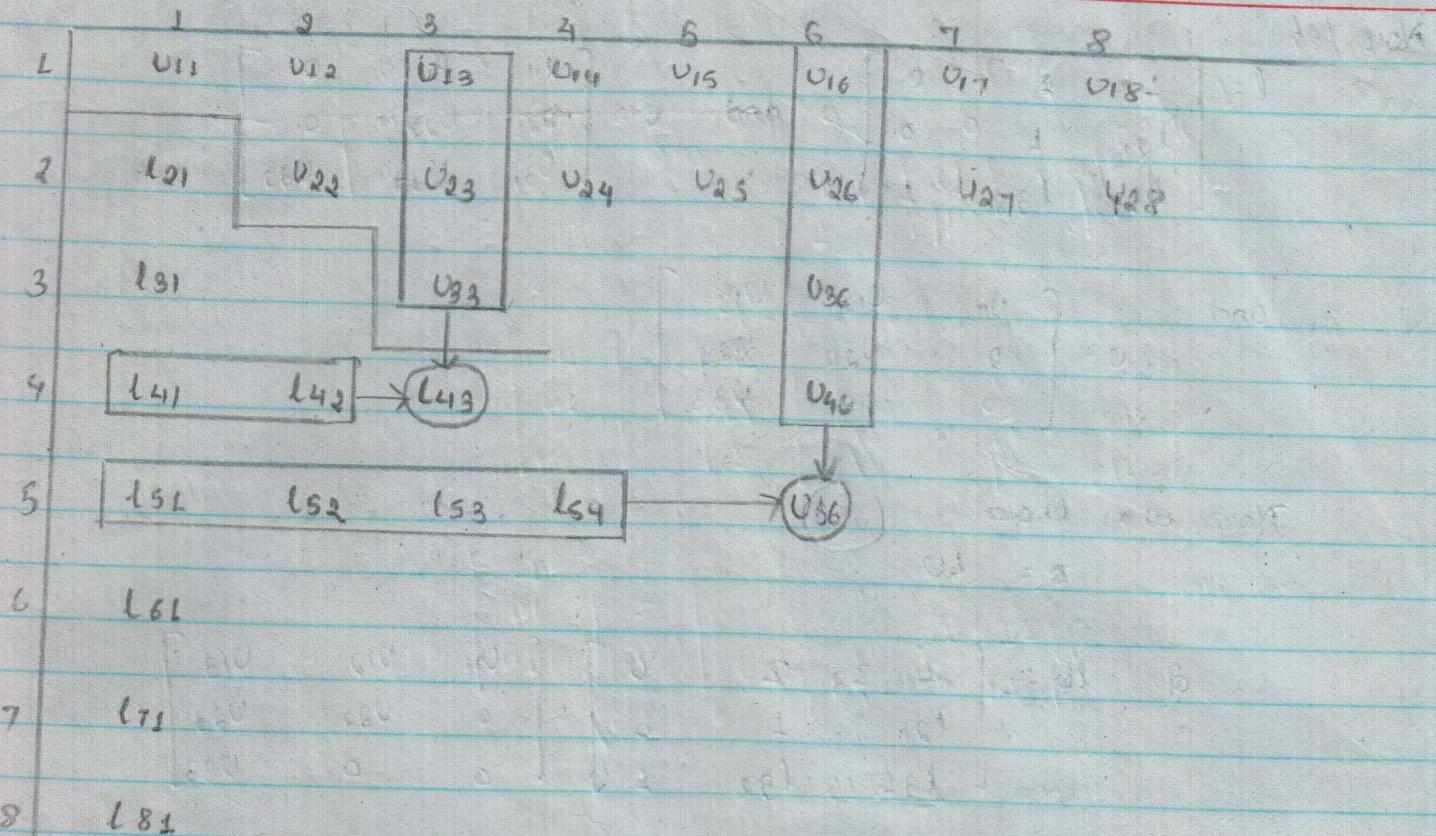
$$= \frac{1}{25} //$$

Hence

$$L = \begin{bmatrix} 1 & 0 & 0 \\ \frac{1}{2} & 1 & 0 \\ \frac{31}{50} & -\frac{17}{25} & 1 \end{bmatrix} \quad \& \quad U = \begin{bmatrix} 60 & 107 & 36 \\ 0 & \frac{1}{2} & 2 \\ 0 & 0 & \frac{1}{25} \end{bmatrix}$$

Note:

for computing any element, we needs the values of elements in the previous columns as well as the values of elements in the column above that element. as illustrated in the figure given below.



Pictorial view of Doolittle algorithm for LU decomposition

Solve the system by using Doolittle LU decomposition method.

$$3x_1 + 2x_2 + x_3 = 10$$

$$2x_1 + 3x_2 + 2x_3 = 14$$

$$x_1 + 2x_2 + 3x_3 = 14$$

Solution,

Given equations are,

$$3x_1 + 2x_2 + x_3 = 10$$

$$2x_1 + 3x_2 + 2x_3 = 14$$

$$x_1 + 2x_2 + 3x_3 = 14$$

So, the matrix A is given by,

$$A = \begin{bmatrix} 3 & 2 & 1 \\ 2 & 3 & 2 \\ 1 & 2 & 3 \end{bmatrix}$$

Now let

$$L = \begin{bmatrix} 1 & 0 & 0 \\ l_{21} & 1 & 0 \\ l_{31} & l_{32} & 1 \end{bmatrix} \quad \text{and} \quad U = \begin{bmatrix} u_{11} & 0 & 0 \\ u_{21} & u_{22} & 0 \\ u_{31} & u_{32} & u_{33} \end{bmatrix}$$

$$\text{and} \quad U = \begin{bmatrix} u_{11} & u_{12} & u_{13} \\ 0 & u_{22} & u_{23} \\ 0 & 0 & u_{33} \end{bmatrix}$$

Now we know

$$A = LU$$

$$\text{So } LU = \begin{bmatrix} 1 & 0 & 0 \\ l_{21} & 1 & 0 \\ l_{31} & l_{32} & 1 \end{bmatrix} \begin{bmatrix} u_{11} & u_{12} & u_{13} \\ 0 & u_{22} & u_{23} \\ 0 & 0 & u_{33} \end{bmatrix}$$

$$= \begin{bmatrix} u_{11} & u_{12} & u_{13} \\ l_{21}u_{11} & l_{21}u_{12} + u_{22} & l_{21}u_{13} + u_{23} \\ l_{31}u_{11} & l_{31}u_{12} + l_{32}u_{22} & l_{31}u_{13} + l_{32}u_{23} + u_{33} \end{bmatrix}$$

Hence,

$$u_{11} = 3$$

$$u_{12} = 2$$

$$u_{13} = 1$$

and

$$l_{21}u_{11} = 2$$

$$\text{or } l_{21} \cdot 3 = 2$$

$$\text{or, } l_{21} = \frac{2}{3}$$

$$\text{and } l_{21}u_{12} + u_{22} = 3$$

$$\frac{2}{3} \times 2 + u_{22} = 3$$

$$\text{or, } u_{22} = 3 - \frac{4}{3}$$

and

$$l_{31}u_{11} = 1$$

$$\text{or } l_{31} \cdot 3 = 1$$

$$\text{or, } l_{31} = \frac{1}{3}$$

$$= \frac{5}{3}$$

$$\text{Set sum} = \sum_{j=1}^{i-1} a_{ij} z_j \quad \left. \begin{array}{l} \\ \end{array} \right\} \text{forward substitution}$$

Set $z_i = b_i - \text{sum}$

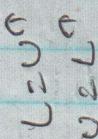
repeat i .

6. Set $x_n = \frac{z_n}{a_{nn}}$

7. for $i = n-1$ to 1

$$\text{Set sum} = \sum_{j=i+1}^n a_{ij} x_j$$

repeat i



8. Write result.

* Cholesky method :-

when A is symmetric, the LU decomposition can be modified so that, the upper factor is the transpose of the lower one or vice-versa. That is we can factorize A such that,

$$A = LL^T$$

$$\text{or, } A = LUL^T \quad \textcircled{1}$$

Similar to Doolittle decomposition by multiplying the terms of eqn $\textcircled{1}$ & setting them equal to each other the following recurrence relation can be obtain.

$$U_{ij} = \sqrt{a_{ii} - \sum_{k=1}^{i-1} U_{ki}^2} \quad \text{for } (i=2 \text{ to } n).$$

$$U_{ij} = \frac{1}{U_{ii}} \left[a_{ij} - \sum_{k=1}^{i-1} U_{ki} U_{kj} \right] (j < i)$$

The decomposition is called Cholesky's method or the method of square roots.

* Algorithm (cholesky's factorization)

1. Given n, A
2. set $U_{11} = \sqrt{A_{11}}$
3. set $U_{1j}^0 = A_{1j} / U_{11}$
4. for $j = 2$ to n
 - for $i = 2$ to j
 - sum \hat{A}_{ij}
 - for $k = 1$ to $i-1$
 - sum = sum - $U_{ki}^0 U_{kj}^0$
 - repeat k .

set $U_{ij}^0 = \text{sum} / U_{ii}^0$ if $i < j$

set $U_{jj}^0 = \sqrt{\text{sum}}$ if $i = j$

repeat i

repeat j .

5. End of factorization.

Q. Factorize the matrix

$$A = \begin{bmatrix} 1 & 2 & 3 \\ 2 & 8 & 22 \\ 3 & 22 & 82 \end{bmatrix} \quad \text{using Cholesky algorithm.}$$

$$\Rightarrow \text{Given, } A = \begin{bmatrix} 1 & 2 & 3 \\ 2 & 8 & 22 \\ 3 & 22 & 82 \end{bmatrix}$$

then,

$$U^T U = A$$

So,

$$U^\dagger U = \begin{bmatrix} U_{11} & 0 & 0 \\ U_{12} & U_{22} & 0 \\ U_{13} & U_{23} & U_{33} \end{bmatrix} \begin{bmatrix} U_{11} & U_{12} & U_{13} \\ 0 & U_{22} & U_{23} \\ 0 & 0 & U_{33} \end{bmatrix}$$

$$\Rightarrow \begin{bmatrix} U_{11}^2 & U_{11}U_{12} & U_{11}U_{13} \\ U_{12}U_{11} & U_{12}^2 + U_{22}^2 & U_{12}U_{13} + U_{22}U_{23} \\ U_{13}U_{11} & U_{13}U_{12} + U_{23}U_{22} & U_{13}^2 + U_{23}^2 + U_{33}^2 \end{bmatrix} = \begin{bmatrix} 1 & 2 & 3 \\ 2 & 8 & 22 \\ 0 & 22 & 82 \end{bmatrix}$$

Now,

$$\Rightarrow U_{11} = 1 \rightarrow U_{11} = 1$$

$$\Rightarrow U_{12}U_{11} = 2 \rightarrow U_{12} = 2/1 = 2$$

$$\Rightarrow U_{13}U_{11} = 3 \rightarrow U_{13} = 3$$

$$\Rightarrow U_{11}U_{12} = 2 \rightarrow U_{12} = 2$$

$$\Rightarrow U_{12}^2 + U_{22}^2 = 8 \rightarrow U_{22} = \sqrt{8 - U_{11}^2} = \sqrt{8 - 2^2} = 2$$

$$\Rightarrow U_{23}U_{12} + U_{23}U_{22} = 22 \Rightarrow U_{23} = (22 - U_{13}U_{12})/U_{22} \\ = (22 - 3 \times 2)/2 \\ = \frac{16}{2}$$

$$= 8$$

$$\Rightarrow U_{11}U_{13} = 3 \rightarrow U_{13} = 3$$

$$\Rightarrow U_{13}^2 + U_{23}^2 + U_{33}^2 = 82$$

$$\Rightarrow U_{33} = \sqrt{82 - 64 - 9}$$

$$= \sqrt{9} \\ = 3$$

$$U = \begin{bmatrix} 1 & 2 & 3 \\ 0 & 2 & 8 \\ 0 & 0 & 3 \end{bmatrix}, U^\dagger = \begin{bmatrix} 1 & 0 & 0 \\ 2 & 2 & 0 \\ 3 & 8 & 3 \end{bmatrix}$$

Any

~~120~~ 120

+ Iterative solution of linear Equations:

Direct method which we have studied previously have some problems when the system grows larger or when most of the coefficients are zero. They require large no of floating points operations & therefore it consumes time as well as severely affect the accuracy of the solution due to round off errors. In such case iterative method provides an alternative. For example ill conditioned system can be solved by iterative methods without facing the problem of round off errors.

Following iterative methods are studied.

122

obtain the solⁿ of following system using Jacobi iteration.

$$2x_1 + 3x_2 + x_3 = 5$$

$$3x_1 + 5x_2 + 2x_3 = 15$$

$$8x_1 + x_2 + 4x_3 = 8$$

Solution :-

First solve the equation for unknowns on the diagonal. That means,

$$x_1 = \frac{5 - x_2 - x_3}{2}$$

$$x_2 = \frac{15 - 3x_1 - 2x_3}{5}$$

$$x_3 = \frac{8 - 2x_1 - x_2}{4}$$

If we assume the initial values of $x_1, x_2, x_3 = 0$ we get,

$$x_1^{(1)} = \frac{5}{2} = 2.5_{//}$$

$$x_2^{(1)} = \frac{15}{5} = 3_{//}$$

$$x_3^{(1)} = \frac{8}{4} = 2_{//}$$

For the 2nd iteration we have, $x_1 = 2.5, x_2 = 3, x_3 = 2$

$$x_1^{(2)} = \frac{5 - 3 - 2}{2}$$

$$= 0.5 = 0_{//}$$

$$x_2^{(2)} = \frac{15 - 3 \times 2.5 - 2 \times 2}{5}$$

$$= \frac{8.5}{5} = 0.7$$

$$x_3^{(2)} = \frac{8 - 2 \times 2.5 - 3}{4}$$

$$= 0_{//}$$

123

for the 3rd iteration we have $x_1 = 0.7, x_2 = 0, x_3 = 0$

$$x_1^{(3)} = \frac{5 - 0.7 - 0}{2}$$

$$= 2.015$$

$$x_2^{(3)} = \frac{15 - 3 \times 0 - 2 \times 0}{5}$$

$$= 3.11$$

$$x_3^{(3)} = \frac{8 - 2 \times 0 - 0.7}{4}$$

$$= 1.9825$$

for 4th iteration we have $x_1 = 2.015, x_2 = 3, x_3 = 1.9825$

$$x_1^{(4)} = \frac{5 - 3 - 2}{2}$$

$$= 0.11$$

$$x_2^{(4)} = \frac{15 - 3 \times 2.015 - 2 \times 1.9825}{5}$$

$$= 0.0777$$

$$x_3^{(4)} = \frac{8 - 2 \times 2.015 - 1}{4}$$

$$= 0.04875$$

124

for 5th iteration, we have, $x_1 = 0$, $x_2 = 0.77$, $x_3 = 0.46875$
Hence,

$$x_1^{(5)} = \frac{5 - 0.77 - 0.46875}{4} \\ = \underline{1.081375}, 2.0349375$$

$$x_2^{(5)} = \frac{15 - 3x_0 - 2x_1^{(5)} - 0.46875}{5} \\ = \underline{2.081325}$$

$$x_3^{(5)} = \frac{8 - 2x_0 - 0.746875}{4} \\ = \underline{1.08828}$$

Hence after 6th iteration, the values of x_1, x_2, x_3 are

$$x_1 = 2.0349375$$

$$x_2 = 2.081325$$

$$x_3 = 1.08828125$$

Algorithm for Jacobi Iteration method.

- ① obtain n, a_{ij} , and b_i values
- ② set $x_{0i} = b_i/a_{ii}$ for $i = 1, \dots, n$
- ③ set key = 0
- ④ for $i = 1, 2, \dots, n$
 - ① set sum = b_i
 - ② for $j = 1, 2, \dots, n$ ($j \neq i$), set sum = sum - $a_{ij}x_{0j}$
repeat j ;
 - ③ set $x_i^0 = \text{sum}/a_{ii}$
 - ④ if $\text{key} = 0$ then

$$\text{if } \left| \frac{x_i^0 - x_{0i}}{x_i^0} \right| > \text{Error} \text{ then}$$

set key = 1;

Repeat i ;
 - ⑤ if $\text{key} = 1$ then,
set $x_{0i} = x_i^0$
goto step 3
- ⑥ write Results.

Gauss-Seidel method.

It is an improved version of Jacobi iteration method.
In Jacobi method we began with the initial values $x_1^{(0)}$, $x_2^{(0)}, \dots, x_n^{(0)}$ and obtain the next approximation $x_1^{(1)}$, $x_2^{(1)}, \dots, x_n^{(1)}$.

Note that in computing $x_2^{(1)}$ we use $x_1^{(0)}$ but not $x_1^{(1)}$ which has just been computed.

Since at this point both $x_1^{(0)}$ and $x_1^{(1)}$ are available, we can use $x_1^{(1)}$ which is a better approximation for computing $x_2^{(1)}$.

Similarly for computing $x_3^{(1)}$ we use $x_1^{(1)}$ & $x_2^{(1)}$. Along with $x_1^{(0)}, \dots, x_n^{(0)}$. This idea is extended to all subsequent computation & this approach is called Gauss Seidel method.

Thus the Gauss Seidel method uses the most recent values of x as soon as they become available at any point of iteration process. During the $(k+1)^{th}$ iteration of Gauss Seidel method, $x_i^{(k)}$ takes the form:

$$x_i^{(k+1)} = b_i - a_{i1}^{(k)} x_1^{(k+1)} - \dots - a_{i(i-1)}^{(k)} x_{i-1}^{(k+1)} + a_{i(i+1)}^{(k)} x_{i+1}^{(k+1)}$$

$$+ \dots + a_{in}^{(k)} x_n^{(k)}$$

\downarrow
 b_i

following figure illustrates pictorially the difference between Jacobian & Gauss Seidel method

$$\boxed{\begin{aligned} x_1^{(0)} &= (b_1 - a_{12} x_2 - a_{13} x_3) / a_{11} \\ x_2^{(0)} &= (b_2 - a_{21} x_1 - a_{23} x_3) / a_{22} \\ x_3^{(0)} &= (b_3 - a_{31} x_1 - a_{32} x_2) / a_{33} \end{aligned}}$$

$$\begin{aligned} x_1^{(1)} &= (b_1 - a_{12} \overset{\downarrow}{x}_2^{(0)} - a_{13} x_3^{(0)}) / a_{11} \\ x_1^{(2)} &= (b_2 - a_{21} x_1^{(0)} - a_{23} x_3^{(0)}) / a_{22} \\ x_1^{(3)} &= (b_3 - a_{31} x_1^{(0)} - a_{32} \overset{\downarrow}{x}_2^{(0)}) / a_{33} \end{aligned}$$

fig : Jacobi method;

$$\boxed{\begin{aligned} x_1 &= (b_1 - a_{12} x_2 - a_{13} x_3) / a_{11} \\ x_2 &= (b_2 - a_{21} x_1 - a_{23} x_3) / a_{22} \\ x_3 &= (b_3 - a_{31} x_1 - a_{32} \overset{\downarrow}{x}_2) / a_{33} \end{aligned}}$$

fig :- Gauss Seidel method.

Obtain the solution of given equation using Gauss Seidal method.

$$2x_1 + x_2 + x_3 = 5$$

$$8x_1 + 5x_2 + 2x_3 = 15$$

$$2x_1 + x_2 + 4x_3 = 8$$

Sol^b,

first we solve the equation for unknowns on diagonal, that means,

$$x_1 = \frac{5 - x_2 - x_3}{2}$$

$$x_2 = \frac{15 - 3x_1 - 2x_3}{5}$$

$$x_3 = \frac{8 - 2x_1 - x_2}{4}$$

let the initial values of x_2 & $x_3 = 0$ so

$$x_1 = \frac{5 - 0 - 0}{2}$$

$$= 2.5 //$$

$$x_2 = \frac{15 - 3(2.5) \times 2.5 - 2 \times 0}{5}$$

$$= 1.5 //$$

$$x_3 = \frac{8 - 2 \times 2.5 - 1.5}{4}$$

$$= \frac{1.5}{4}$$

$$= 0.375 //$$

In second iteration

$$x_1 = \frac{5 - 1.5 - 0.375}{2}$$

$$= 1.55$$

128

$$x_2 = \frac{15 - 3 \times 10.55 - 0.42 \times 0.0375}{5}$$
$$= 2.031099$$

$$x_3 = \frac{8 - 2 \times 10.55 - 10.99}{4}$$
$$= 0.072495$$

for third iteration $x_2 = 1.99, x_3 = 0.072495$

Hence

$$x_1 = \frac{5 - 10.99 - 0.072495}{2}$$
$$= 1.01675$$

$$x_2 = \frac{15 - 3 \times 10.1675 - 2 \times 10.99}{5}$$
$$= 1.05315$$

$$x_3 = \frac{8 - 2 \times 1.01675 - 1.05315}{4}$$
$$= 0.033375$$

Now for 4th iteration, $x_2 = 1.05315, x_3 = 0.033375$

then

$$x_1 = \frac{5 - 1.05315 - 0.033375}{2}$$

$$= 1.02173625$$

~~using this we obtain the following~~

$$x_2 = \frac{15 - 3 \times 10.2175625 - 2 \times 10.033375}{5}$$

$$= 10.85611$$

$$x_3 = \frac{8 - 2 \times 10.2175625 - 10.856}{4}$$

$$= 0.0927211$$

for 5th iteration, $x_2 = 10.856, x_3 = 0.09272$,

then

$$x_1 = \frac{5 - 10.856 - 0.09272}{2}$$

$$= 0.608411$$

$$x_2 = \frac{15 - 3 \times 0.608411 - 2 \times 0.09272}{5}$$

$$= 2.026408$$

$$x_3 = \frac{8 - 2 \times (0.608411) - 2.026408}{4}$$

$$= 1.012978$$

Hence after 5th iteration

$$x_1 = 0.608411$$

$$x_2 = 2.026408$$

$$x_3 = 1.012978$$

Numerical Differentiation and Integration:

Numerical Differentiation,

It is the process of calculating the value of the derivative of the function at some assigned value of n from the given set of values (x_i, y_i) . To compute $\frac{dy}{dx}$, we first replace the exact relation $y = f(x)$ by the best interpolating polynomial $y = p(x)$ and then differentiate the latter as many times as we desire.

Differentiation is one of the most important concepts in calculus which has been used almost everywhere in many fields of mathematics and applied mathematics & engineering.

If the values of x are equispaced and $\frac{dy}{dx}$ is required near the beginning of the table we use Newton's forward formula. If it is required near the end of the table, we use Newton's backward formula. For values near the middle of the table $\frac{dy}{dx}$ is calculated by means of Stirling's or Bessel's formula.

If the values of x are not equispaced, we use Newton's formula to represent the function.

Hence, corresponding to each of the interpolation formula we can derive a formula for finding the derivative.

Derivative from the divide difference table.

Q. Find $f'(10)$ from the following data.

$x :$	8	6	11	27	34
$f(x) :$	-13	23	899	17315	35606

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Constructing Newton's divided difference table we have,

x	$f(x)$	1st diff	2nd diff	3rd diff	4th diff
3	-13	18			
5	23		16	0	
7	899	146.567		1	
11	17315	1026 1026 375	40		0
17	2613		69		
34	85606				

Now,

we have,

$$\begin{aligned}
 f(x) &= q_0 + q_1(x-x_0) + q_2(x-x_0)(x-x_1) + q_3(x-x_0) \\
 &\quad (x-x_1)(x-x_2) + q_4(x-x_0)(x-x_1)(x-x_2)(x-x_3) \\
 &= -13 + q_1(x-3) + 18(x-3)(x-5) + 16(x-3) \\
 &\quad (x-5)(x-11) + q_4(x-3)(x-5)(x-11) \\
 &= -13 + 18x - 84 + 16(x^2 - 5x - 3x + 15) + 16 \\
 &\quad + 1(x^2 - 5x - 3x + 15)(x-11) \\
 &= -13 + 18x + 54 + 16x^2 - 80x - 48x + 240 \\
 &\quad + (x^3 - 5x^2 - 3x^2 + 15x - 11x^2 + 55x + 33x) + 16 \\
 &= x^3 - 3x^2 - 7x + 8
 \end{aligned}$$

Now

$$\begin{aligned}
 f'(x) &= 3x^2 - 6x - 7 \\
 f'(10) &= 3(10)^2 - 6 \times 10 - 7 \\
 &= 233
 \end{aligned}$$

Derivative using forward difference formula

Consider Newton's forward difference formula

$$y = y_0 + u \Delta y_0 + \frac{\Delta(u-1)}{2!} \Delta^2 y_0 + \frac{u(u-1)(u-2)}{3!} \Delta^3 y_0 + \dots \quad (1)$$

$$\text{where } x = x_0 + uh \quad \dots \quad (2)$$

Then,

$$\frac{dy}{dx} = \frac{dy}{du} \times \frac{\partial u}{\partial x}$$

$$= \frac{1}{h} \left[\Delta y_0 + \frac{2u-1}{2} \Delta^2 y_0 + \frac{3u^2 - 6u + 3}{6} \Delta^3 y_0 + \dots \right] \quad (3)$$

This formula can be used for computing the values of dy/dx for non tabular values of x . For tabular values of x , the formula takes a simple form; for by setting $x = x_0$, we obtain.

$$u = 0 \text{ from eqn (2)}$$

Hence eqn (3) gives

$$\left[\frac{dy}{dx} \right]_{x=x_0} = \frac{1}{h} \left[\Delta y_0 - \frac{1}{2} \Delta^2 y_0 + \frac{1}{3} \Delta^3 y_0 + \dots \right] \quad (4)$$

Differentiating eqn (4) once again we get,

$$\frac{d^2y}{dx^2} = \frac{1}{h^2} \left[\Delta^2 y_0 + \frac{6u-6}{6} + \frac{12u^2 - 36u + 36}{24} \Delta^4 y_0 + \dots \right] \quad (5)$$

from which we can obtain:

$$\left[\frac{d^2y}{dx^2} \right]_{x=x_0} = \frac{1}{h^2} \left[\Delta^2 y_0 - \Delta^3 y_0 + \frac{11}{12} \Delta^4 y_0 - \dots \right] \quad (6)$$

Formula for higher derivatives may be obtained by substituting successive differentiation.

From the following table of values of x & y obtain $\frac{dy}{dx}$

x	1.0	1.2	1.4	1.6	1.8	2.0	2.2
y	2.7183	3.3202	4.0552	4.9530	6.0496	7.3891	9.0250

60th

constructing the forward difference table, we get.

x	y	Δy_0	$\Delta^2 y_0$	$\Delta^3 y_0$	$\Delta^4 y_0$	$\Delta^5 y_0$	$\Delta^6 y_0$
1.0	2.7183						
1.2	3.3202	-23.868*					
1.4	4.0552	0.7351*	-24.598				
1.6	4.9530	0.1627*	-24.4353	24.4714			
1.8	6.0496	0.8958	0.0361*	-24.4634	24.4648	v-cdf	
2.0	7.3891	1.0966	0.1988	0.008*	0.0014*		
2.2	9.0250	1.3395	0.2429	0.0094	0.0014*		x - backward
		1.63596	0.2964	0.0595			

Here,

$$x_0 = 1.2$$

$$y_0 = 3.3202$$

$$h = 0.2$$

$$\left[\frac{dy}{dx} \right]_{x=1.2} = \frac{1}{0.2} \left[0.7351 - \frac{1}{2} (0.1627) + \frac{1}{3} (0.0361) - \frac{1}{4} (0.0080) \right.$$

$$\left. + \frac{1}{5} (0.0014) \right]$$

$$= 3.3205 //$$

$$\left[\frac{d^2y}{dx^2} \right]_{x=1.2} = \frac{1}{(0.2)^2} \left[\Delta^2 y_0 + \Delta^3 y_0 \cdot \frac{11}{12} \Delta^4 y_0 - \frac{5}{6} \Delta^5 y_0 + \frac{137}{180} \Delta^6 y_0 \dots \right]$$

$$= \frac{1}{(0.2)^2} \left[0.01627 - 0.0361 + \frac{11}{12} 0.0008 - \frac{5}{6} 0.00014 \right]$$

$$= -1.30319 \dots$$

Numerical Backward difference formula.

$$\left[\frac{dy}{dx} \right]_{x=x_n} = \frac{1}{h} \left[\nabla y_n + \frac{1}{2} \nabla^2 y_n + \frac{1}{3} \nabla^3 y_n \dots \right]$$

and,

$$\left[\frac{d^2y}{dx^2} \right]_{x=x_n} = \frac{1}{h^2} \left[\nabla^2 y_n + \nabla^3 y_n + \frac{11}{12} \nabla^4 y_n + \frac{5}{6} \nabla^5 y_n \dots \right]$$

central Difference formula:

① starting's formula.

$$\left[\frac{dy}{dx} \right]_{x=x_0} = \frac{1}{h} \left[\frac{\Delta y_{-1} + \Delta y_0}{2} - \frac{1}{6} \frac{\Delta^3 y_{-2} + \Delta^3 y_{-1} + \Delta^3 y_{-3} - \Delta^3 y_0}{2} \right]$$

$$\therefore \left[\frac{d^2y}{dx^2} \right]_{x=x_0} = \frac{1}{h^2} \left[\Delta^2 y_{-1} - \frac{1}{12} \Delta^4 y_{-2} + \frac{1}{90} \Delta^6 y_{-3} \dots \right]$$

Q) calculate the first & second derivative of the function tabulated in the preceding example at point $x=1.2$ and also dy/dx at $x=2.2$.

Sol/

$$\text{Here } x_0 = 2.0$$

$$y_0 = 9.0250$$

$$\& h = 0.2$$

By using Newton's backward formula,

$$\left[\frac{dy}{dx} \right]_{x=2.2} = \frac{1}{0.2} \left[1.6359 + \frac{1}{2} 0.2964 + \frac{1}{3} 0.0535 + \frac{1}{4} 0.0094 \right. \\ \left. + \frac{1}{5} 0.0014 + \frac{1}{6} 24.04648 \right] \\ = 36.7911$$

$$\left[\frac{d^2y}{dx^2} \right]_{x=2.2} = \frac{1}{(0.2)^2} \left[0.2964 + 0.0535 + \frac{11}{12} 0.0094 + \frac{5}{6} 0.0014 \right]$$

$$= \frac{1}{0.04} \left[0.2964 + 0.0535 + 0.0086 + 0.00116 \right]$$

$$= \frac{1}{0.04} (0.3596)$$

$$= \frac{0.3596}{0.04}$$

$$= 8.9915$$

138

Q) Find $\frac{dy}{dx}$ & $\frac{d^2y}{dx^2}$ at $x=1.6$ for the tabulated function of above example.

Sol:

Hence the value lies between or in central part we use central difference formula & choosing $x_0 = 1.6$ we get,

$$\left[\frac{dy}{dx} \right]_{x=1.6} = \frac{1}{0.2} \left[\frac{0.08978 + 1.0699 - \frac{1}{6} \cdot 0.0361 + 0.0441}{2} + \frac{1}{80} (-24.4364 + 0.0014) \right]$$

$$= \frac{1}{0.2} \left[0.98385 - 0.00668 + (-0.40725) \right]$$

$$= 20.8496 //$$

And

$$\left[\frac{d^2y}{dx^2} \right]_{x=1.6} = \frac{1}{0.04} \left[0.01988 - \frac{1}{12} (0.0080) + \frac{1}{90} (0.0001) \right] \\ [24.04648]$$

$$= 11.74954 //$$

The table below gives the values of distance travelled by a car at various time interval during the initial running.

Time (t) (sec) 5 6 7 8 9 10

Distance (S) (km) 10.0 14.0 19.0 25.5 32.0

estimate the velocity at time $t=5, t=7$ & $t=9$

Solution

//

t	s	Δs_0	$\Delta^2 s_0$	$\Delta^3 s_0$	$\Delta^4 s_0$
5	10.0				
	4.05				
6	14.05		0.05		
	6.0			0.05833	
7	19.05		1.0	-0.05833	-0.00000
	6.05				
8	25.05		0.05		
	6.05				
9	32.00				

for time $t = 5$ we use forward difference formula,
then,

$$\left[\frac{ds}{dt} \right]_{t=5} = \frac{1}{h} \left[\Delta s_0 - \frac{1}{2} \Delta^2 s_0 + \frac{1}{3} \Delta^3 s_0 + \frac{1}{4} \Delta^4 s_0 \right]$$

$$= \frac{1}{1} \left[4.05 - \frac{1}{2} (0.05) + \frac{1}{3} (0.05) - \frac{1}{4} (0) \right]$$

$$= 4.05 - 0.025 + 0.01667 + 0.025$$

$$= 4.06667 //$$

for time $t = 7$ we use central difference formula,

$$\left(\frac{ds}{dt} \right)_{t=7} = \frac{1}{h} \left[\frac{\Delta y_1 + \Delta y_0}{2} - \frac{1}{6} \Delta^3 y_2 + \Delta^3 y_1 \right]$$

$$= \frac{1}{1} \left[\frac{6.05 + 6.0}{2} - \frac{1}{6} \cdot \frac{0.05 + (-0.05)}{2} \right]$$

$$\left[\frac{11}{2} - 0 \right]$$

$$= 5.5 //$$

for time $t=9$ we use backward difference formula,

$$\begin{aligned} \left(\frac{dy}{dt} \right)_{t=9} &= \frac{1}{h} \left[\Delta y_n + \frac{1}{2} \Delta^2 y_n + \frac{1}{3} \Delta^3 y_n + \frac{1}{4} \Delta^4 y_n \right] \\ &= \frac{1}{3} \left[6.5 + \frac{1}{2} \times 0.05 + \frac{1}{3} [-0.05] + \frac{1}{4} (-1) \right] \\ &= 6.5 + 0.025 - 0.01667 - 0.025 \\ &= 6.333 // \end{aligned}$$

maxima and minima of tabulated function:-

It is known that the maximum & minimum value of a function can be found by equating the 1st derivative to 0 & solving for variable. The same procedure can be applied to determine the maxima & minima of tabulated function.

Consider Newton's forward interpolation as

$$y = y_0 + p\Delta y_0 + \frac{p(p-1)}{2} \Delta^2 y_0 + \frac{p(p-1)(p-2)}{3!} \Delta^3 y_0 + \dots \quad (1)$$

where,

$$x = x_0 + ph.$$

Differentiating this with respect to p we get,

$$\frac{dy}{dp} = \Delta y_0 + \frac{2p-1}{2} \Delta^2 y_0 + \frac{3p^2 - 6p + 2}{6} \Delta^3 y_0 + \dots \quad (2)$$

for maxima & minima,

$$\frac{dy}{dp} = 0$$

Hence equating the RHS of eqn (ii) to 0 & retaining only upto 3rd difference, we obtain,

$$\Delta y_0 + \frac{2p-1}{4} \Delta^2 y_0 + \frac{3p^2 - 6p + 2}{6} \Delta^3 y_0 = 0$$

$$\text{or, } \left(\frac{1}{2} \Delta^3 y_0 \right) p^2 + (\Delta^2 y_0 - \Delta^3 y_0) p + \left(\Delta y_0 - \frac{1}{2} \Delta^2 y_0 + \frac{1}{3} \Delta^3 y_0 \right) = 0$$

Substituting the value of Δy_0 , $\Delta^2 y_0$ & $\Delta^3 y_0$ from the difference table, we solve this quadratic for p , then the corresponding values of x are given by

$$x = x_0 + ph$$

at which y is maximum or minimum.

From the table below, for what values of x , y is minimum? also find this value of y .

x	3	4	5	6	7	8
y	0.205	0.240	0.259	0.262	0.250	0.224

Soln,

The difference table is as follows

from the table, we get,

$$x_0 = 3$$

$$y_0 = 0.205$$

$$\Delta y_0 = 0.085$$

$$\Delta^2 y_0 = -0.016$$

$$\Delta^3 y_0 = 0$$

Therefore, Newton's forward formula given

$$\begin{aligned} y &= y_0 + p \Delta y_0 + \frac{p(p-1)}{2!} \Delta^2 y_0 + \frac{p(p-1)(p-2)}{3!} \Delta^3 y_0 \\ &= 0.205 + p \times 0.085 + \frac{p(p-1)}{2} (-0.016) \\ &= 0.205 + 0.085p + \frac{(p^2-p)}{2} (-0.016) \end{aligned}$$

Differentiating with respect to p we have

$$\frac{dy}{dp} = 0.085 + \frac{2p-1}{2} (-0.016)$$

for maxima or minima,

$$\frac{dy}{dp} = 0$$

Hence

$$0.085 + \frac{2p-1}{2} (-0.016) = 0$$

$$\text{Or, } 0.085 - 0.016p + \frac{0.016}{2} = 0$$

$$\text{Or, } 0.085 - 0.016p + 0.008 = 0$$

$$\text{Or, } 0.016p = 0.093$$

$$p = 0.6875$$

we know,

$$\begin{aligned} x &= x_0 + ph \\ &= 3 + 2.6875 \times 1 \\ &= 5.6875 // \end{aligned}$$

Hence y is minimum when the value of x is 5.6875

Now putting the obtained values in eqn ① we get,

$$y = y_0 + pA y_0 + \frac{p(p-1)}{2} A^2 y_0$$

$$= 0.205 + 2.6875 \times 0.085 + \frac{2.6875(2.6875-1)}{2} \times 0.016$$

$$= 0.205 + 0.0940625 + (-0.03628125)$$

$$= 0.2990625 - 0.03628125$$

$$= 0.26278125 //$$

Numerical Integration

The process of evaluating a definite integral from a set of tabulated values of the integrand $f(x)$ is called numerical integration. This process when applied to a function of single variable is known as quadrature.

The problem of numerical integration like that of numerical differentiation is solved by representing $f(x)$ by an interpolation formula $P_n(x)$, and then integrating it between the given limits, thus

$$I = \int_a^b f(x) dx \approx \int_0^b p_n(x) dx$$

Also a definite integral of the form $I = \int_a^b f(x) dx$ can be treated as area under

the curve $y = f(x)$ enclosed between the limits $x=a$, and $x=b$. This is graphically illustrated in the figure below.

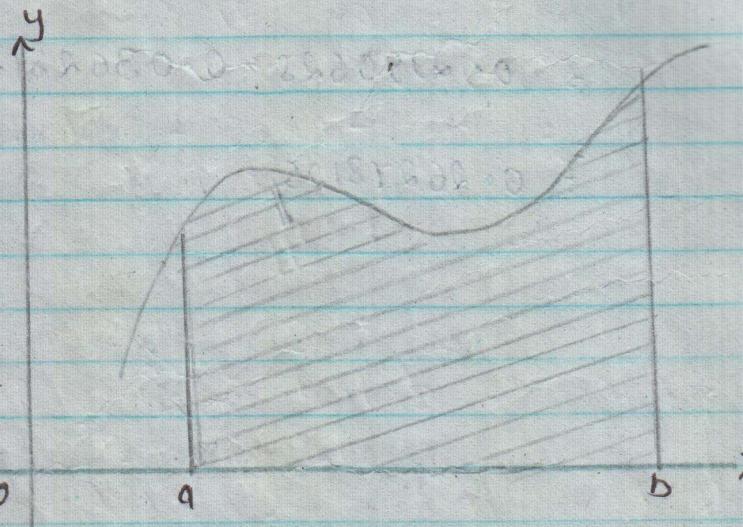


fig: Graphical representation of integral of a function.

Newton-Cotes quadrature formula:

Newton-Cotes formula is the most popular & widely used numerical integration formula. The derivation is based on polynomial interpolation. The limits of integration a & b lie within the interval x_0 & x_n . Then the formula is referred to as closed form. They include

- (i) Trapezoidal rule (two-points formula)
- (ii) Simpson's $\frac{1}{3}$ rule (three-points formula)
- (iii) Simpson's $\frac{8}{3}$ rule (four-points formula)
- (iv) Boole's rule (five-points formula)

All these rules can be formulated using either Newton's or Lagrange interpolation polynomial for approximating the function $f(x)$. Here we use Newton's Gregory forward formula which is given as,

$$P_n(s) = f_0 + \frac{\Delta f_0}{\Delta x} s + \frac{\Delta^2 f_0}{\Delta x^2} \frac{s(s-1)}{2!} + \dots \quad (1)$$

$$= T_0 + T_1 + T_2 + \dots + T_n$$

$$\text{where } s = \frac{(x - x_0)}{h}$$

$$\text{if } h = \frac{x_i + 1 - x_i}{2} = \frac{1}{2}$$

Trapezoidal Rule

It is the 1st & simplest rule of Newton's Cotes formula. Since it is two-point formula, it uses the 1st order interpolation polynomial,

$P_1(x)$ for approximating the function $f(x)$.

& assumes $x_0 = a$ & $x_1 = b$.

This is shown in the figure below

144

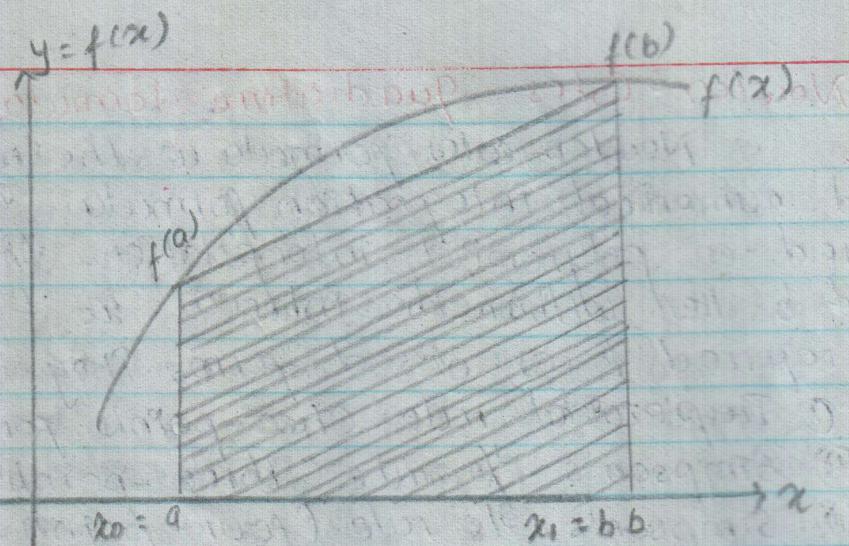


Fig.: Representation of trapezoidal rule.

$$\text{Area} = \frac{f(b) + f(a)}{2} (b - a)$$

Since it is a ~~too~~ point formula, eqn (I) consists of, first two terms T_0 & T_1 . Therefore the integral for trapezoidal rule is given by,

$$\begin{aligned} I_T &= \int_a^b (T_0 + T_1) dx \\ &= \int_a^b T_0 dx + \int_a^b T_1 dx \\ &= I_{T_1} + I_{T_2} \end{aligned}$$

Since T_i are expressed in terms of s & s equals

$$s = (x - x_0)/h$$

we have,

$$dx = h s ds$$

$$x_0 = 0$$

$$x_1 = b$$

if

$$h = x_1 - x_0$$

$$= b - a$$

$$\text{at } x=a, s = \frac{a-x_0}{h}$$

$$= 0/h$$

$$= 0//$$

$$\text{at } x=b, s = \frac{b-a}{h}$$

$$= \frac{1}{h}$$

$$= 1//$$

Then,

$$It_1 = \int_a^b T_0 dx$$

$$= \int_0^1 f_0 h ds$$

$$= hf_0 //$$

$$It_2 = \int_a^b T_1 dx$$

$$= \int_0^1 A f_0 h ds$$

$$= h A f_0 \int_0^1 s ds$$

$$= \frac{h A f_0}{2} //$$

Therefore,

$$It = hf_0 + \frac{h A f_0}{2}$$

$$= h \left[f_0 + \frac{\Delta f_0}{2} \right]$$

$$= h \left[f_0 + \frac{f_1 - f_0}{2} \right]$$

$$= h \left[\frac{2f_0 + f_1 - f_0}{2} \right]$$

$$= h \left[\frac{f_0 + f_1}{2} \right]$$

Since, $f_0 = f(a)$ & $f_1 = f(b)$ we have,

$$It = h \left[\frac{f(a) + f(b)}{2} \right]$$

where $h = b - a$

$$It = \frac{f(a) + f(b)}{2} (b - a)$$

Evaluate the integral

$$I = \int_a^b (x^3 + 1) dx \text{ for the interval,}$$

- (i) (1, 2) (ii) (1, 10.5)

(i) Soln,

$$\text{Given } I = \int_a^b (x^3 + 1) dx$$

here,

$$a = 1$$

$$b = 2$$

$$h = 2 - 1$$

$$= 1/1$$

Part

Note, $f(a) = f(1) = 1^3 + 1$
 $= 2$

$f(b) = f(2) = 2^3 + 1$
 $= 9$

Note,

$$2t = \frac{f(a) + f(b)}{2} (b-a)$$

$$= \frac{2+9}{2} (2-1)$$

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

$$= 5^{\circ} 5\frac{1}{2}$$

(ii) solb,

Here $a = 1$

$$b = 105$$

$$(b-a) = 105 - 1$$

 $= 104$

i, $f(a) = 1^3 + 1$
 $= 2$

$$\therefore f(105) = (105)^3 + 1$$

 $= 40375$

Note, $2t = \frac{f(a) + f(b)}{2} (b-a)$
 $= \frac{2 + 40375}{2} (104)$
 $= 1034375$

(1/3)

Simpson's Rule

In this rule the function $f(x)$ is approximated by a second order polynomial $P_2(x)$ which passes through 3 sampling points as shown in figure.

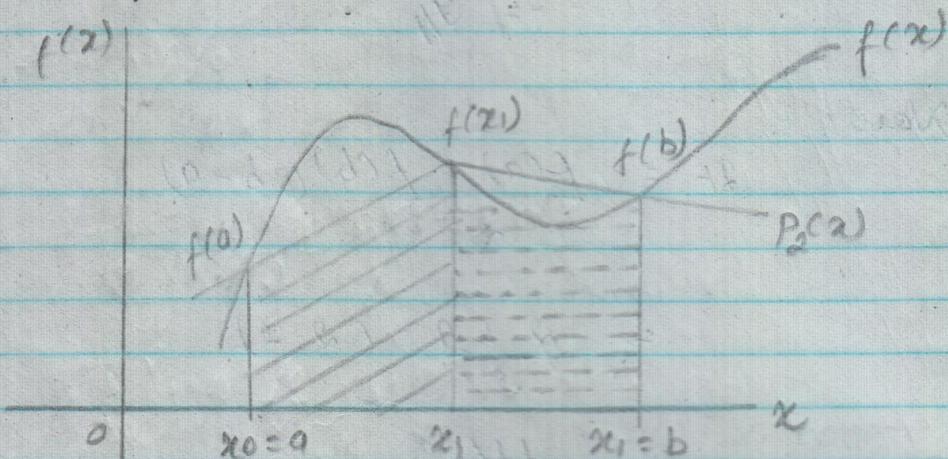


fig: representation of Simpson's 1/3 rule.

Here, the three points including the end points a & b and a mid point c lie between them, i.e

$$x_0 = a$$

$$x_2 = b$$

$$x_1 = \frac{a+b}{2}$$

Therefore, the width of the segment h is given by,

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

The integral for Simpson's 1/3 rule is obtained by integrating in terms of eqn (I) i.e,

$$I_s = \int_a^b P_2(x) dx$$

$$= \int_a^b (f_0 + f_L + f_S) dx$$

$$= \int_a^b f_0 dx + \int_a^b f_L dx + \int_a^b f_S dx$$

$$= I_{S1} + I_{S2} + I_{S3}$$

where,

$$I_{S1} = \int_a^b f_0 dx =$$

$$I_{S2} = \int_a^b \Delta f_0 ds$$

$$I_{S3} = \int_a^b \frac{\Delta^2 f_0}{2} s(s-1) ds$$

$$\text{where, } s = (x - x_0)/h$$

$$dx = h \times ds$$

at,

$$x = a, s = (a - x_0)/h = 0$$

$$x = b, s = (b - x_0)/h$$

$$= (b - a)/h$$

$$= \Delta h/h$$

$$= \Delta h/h$$

Thus,

$$I_{S1} = \int_a^b f_0 dx$$

$$= \int_0^{\Delta h} f_0 h ds$$

$$= \Delta h f_0$$

$$IS_2 = \int_a^b \Delta f_0 s dx$$

$$= \int_0^2 \Delta f_0 sh ds$$

$$= 2h \Delta f_0$$

$$IS_3 = \int_a^b \frac{\Delta^2 f_0}{2} s(s-1) dx$$

$$= \int_0^2 \frac{\Delta^2 f_0}{2} s(s-1) h ds$$

$$= \frac{h}{3} \Delta^2 f_0$$

Therefore,

$$IS = IS_1 + IS_2 + IS_3$$

$$= 2h f_0 + 2h \Delta f_0 + \frac{h}{3} \Delta^2 f_0$$

$$= h (2f_0 + 2\Delta f_0 + \frac{1}{3} \Delta^2 f_0) \dots \textcircled{a}$$

$$= h [2f_0 + 2(f_1 - f_0) + \frac{1}{3} (\Delta f_1 - \Delta f_0)]$$

$$= h [2f_0 + 2f_1 - 2f_0 + \frac{1}{3} [(f_2 - f_1) - (f_1 - f_0)]]$$

$$= h [2f_0 + \frac{1}{3} [f_2 - f_1 - f_1 + f_0]]$$

$$= h \left[\frac{6f_0 + f_2 - 2f_1 + f_0}{3} \right]$$

$$= h \left[\frac{f_2 + 4f_1 + f_0}{3} \right]$$

$$\begin{aligned}
 &= \frac{h}{3} [f_0 + 4f_1 + f_2] \\
 &= \frac{h}{3} [f(a) + 4f(x_1) + f(b)] \\
 &= \frac{(b-a)}{6} \left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b) \right] \\
 &= \frac{(b-a)}{6} \left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b) \right]
 \end{aligned}$$

Evaluate the following integral using Simpson's $\frac{1}{3}$ rule.

$$\textcircled{1} \quad I = \int_{-1}^1 e^x dx \quad (-1, 1)$$

$$\textcircled{2} \quad I = \int_{-1}^{1/2} \sqrt{\sin x} dx \quad (0, 1)$$

\textcircled{3} SOL^b,

$$\text{Here } a = -1$$

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

$$x_1 = \frac{a+b}{2} = \frac{-1+1}{2} = 0$$

$$\text{Now, } I_S = I_{S1} + I_{S2} + I_{S3}.$$

$$\text{for this } f(a) = f(-1) = e^{-1} = 0.3679$$

$$4f\left(\frac{a+b}{2}\right) = 4e^0 = 4$$

$$f(b) = f(1) = e^1 = 2.7183$$

$$\text{So, } \frac{b-a}{3} [f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)]$$

$$= \frac{1}{3} (0.8679 + 4 \times 2.07183)$$

$$= 20.86\% //$$

(ii) ~~graph~~

$$a=0, b=\pi/2 =$$

$$h = \frac{b-a}{2} = \frac{\pi/2 - 0}{2} = 0.7854$$

$$x_1 = \frac{a+b}{2} = \frac{0+\pi/2}{2} = 0.7854$$

$$f(a) = f(0) = \sqrt{\sin 0} = 0$$

$$f(x_1) = f(0.7854) = \sqrt{\sin 0.7854} = 0.11708$$

$$f(b) = f(\pi/2) = \sqrt{\sin \pi/2} = 0.16553$$

Then we know

$$IS = \frac{h}{3} [f(a) + 4f(x_1) + f(b)]$$

$$= \frac{0.7854}{3} [0 + 4 \times 0.11708 + 0.16553]$$

$$= 0.2618 [0.63385]$$

$$= 0.16594 //$$

~~(1/3 + 3x) 1/8 + (1x) 1/8 + (0) 1/8~~

Simpson's 3/8 rule.

Simpson's 3/8 rule is obtained by sampling points by using 3rd order polynomial $P_3(x)$. By using the first four terms of eq 3 (2) & applying the same procedure followed in the previous case, we can show that

$$I_S = \frac{3h}{8} [f(a) + 3f(x_1) + 3f(x_2) + f(b)]$$

$$\text{where } h = \frac{b-a}{3} \quad x_1 = a+h \quad x_2 = a+2h$$

Show eqn is known as Simpson's 3/8 rule.

Q1 Use Simpson's 3/8 rule to evaluate

$$(a) \int_1^2 (x^3 + 1) dx$$

$$(b) \int_0^{\pi/2} \sqrt{\sin x} dx$$

Q1 soln.

$$\text{Given } a=1, b=2$$

$$h = \frac{b-a}{3} = \frac{2-1}{3} = 0.333$$

$$x_1 = a+h = 1+0.333 = 1.333$$

$$x_2 = a+2h = 1+2 \times 0.333 = 1.667$$

Then,

$$f(a) = f(1) = (1^3 + 1) = 2$$

$$f(b) = f(2) = (2^3 + 1) = 9$$

$$f(x_1) = f(1.333) = (1.333^3 + 1) = 2.368$$

$$f(x_2) = f(1.667) = (1.667^3 + 1) = 5.632$$

Now we know,

158

$$IS = \frac{2h}{8} [f(a) + 2f(x_1) + 3f(x_2) + f(b)]$$

$$= \frac{3 \times 0.0233}{8} [2 + 3 \times 8.368 + 3 \times 5.632 + 9]$$

$$= 0.12488 \times 38$$

$$= 4.74541$$

(ii) Soln,

$$\text{Given, } a=0, b=\pi/2$$

$$h = \frac{b-a}{8} = \frac{\pi/2 - 0}{8} =$$

So, 1st point

$$x_1 = 0 + h = \frac{\pi}{16}$$

$$x_2 = 0 + 2h = \frac{\pi}{8}$$

$$x_3 = 0 + 3h = \frac{3\pi}{16}$$

$$x_4 = 0 + 4h = \frac{\pi}{4}$$

$$x_5 = 0 + 5h = \frac{5\pi}{16}$$

$$x_6 = 0 + 6h = \frac{3\pi}{8}$$

$$x_7 = 0 + 7h = \frac{7\pi}{16}$$

Composite Formula for Trapezoidal Rule.

If the range to be integrated is large the trapezoidal rule can be improved by dividing the interval (a, b) into a number of small intervals & applying the same rule to each of these sub intervals. The sum of areas of all the sub-intervals is the integral of the interval (a, b) . This is illustrated in the figure below.

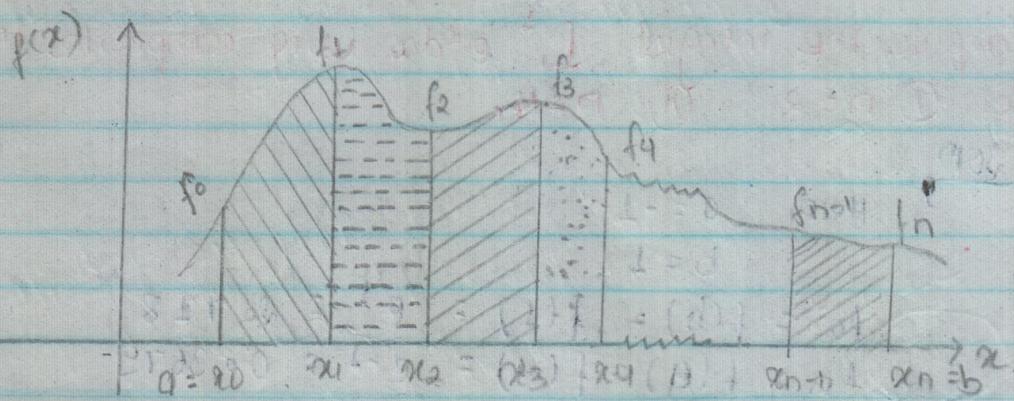


Fig.: Multisegment trapezoidal rule.

In the above figure there are $n+1$ equally spaced sampling points that create n segments of equal width h , given by

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

From the trapezoidal rule, the area of the sub interval with the node x_{i-1} & x_i is given by

$$\begin{aligned} I_i^0 &= \int_{x_{i-1}}^{x_i} p_i(x) dx \\ &= \frac{h}{2} \left[f(x_{i-1}) + f(x_i) \right] \end{aligned}$$

Therefore the total area of all n segments is given by

$$\begin{aligned} \text{Tot} &= \sum_{i=1}^n \frac{h}{2} \left[f(x_{i-1}) + f(x_i) \right] \\ &= \frac{h}{2} [f(x_0) + f(x_1)] + \frac{h}{2} [f(x_1) + f(x_2)] + \frac{h}{2} [f(x_2) \\ &\quad + \dots + f(x_{n-1}) + f(x_n)] \end{aligned}$$

denoting, $f_p = f(x_p)$ & regrouping the terms we get,

$$\begin{aligned} I_{ct} &= \frac{h}{2} (f_0 + f_1) + \frac{h}{2} [f_1 + f_2] + \dots + \frac{h}{2} (f_{n-1} + f_n) \\ &= \frac{h}{2} \left[f_0 + 2 \sum_{i=1}^{n-1} f_i + f_n \right] \end{aligned}$$

which is the general form of trapezoidal rule & is known as composite trapezoidal rule.

Q Compute the integral $\int_{-1}^1 e^x dx$ using composite trapezoidal rule for ① $n=2$ ② $n=4$.

SOP

$$\text{Here, } a = -1$$

$$b = 1$$

$$f_0 = f(b) = f(1) = e^1 = 2.718$$

$$f_n = f(a) = f(-1) = e^{-1} = 0.3679$$

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

$$x_1 = a+h = -1+1 = 0$$

$$\text{then } f(x_1) = f(0) = e^0 = 1$$

Now we know,

$$I_{ct} = \frac{h}{2} \left[f_0 + 2 \sum_{i=1}^{n-1} f(x_i) + f_n \right]$$

$$= \frac{1}{2} \left[2.718 + 2 \times 1 + 0.3679 \right]$$

$$= \frac{6.0869}{2}$$

$$= 3.0439$$