Solution of Nonlinear Equations

In many engineering applications, there are cases when one needs to solve nonlinear algebraic or trigonometric equations or set of equations. These are also common in Civil Engineering problems.

There are several ways of dealing with such nonlinear equations. The solution schemes usually involve an initial guess and successive iterations based on the initial assumption aimed at converging to a value sufficiently close to the exact result. However, the solutions may not always converge to real values and the speed of convergence depends on the accuracy of the solution assumed initially.

Trial and Error Method

Conceptually this is the easiest of all the methods of solving nonlinear equations. It does not require any theoretical background and is particularly convenient with graphical tools. For example, the solution of the nonlinear equation \( f(x) = x^3 - \cos(x) - 2.5 = 0 \) in EXCEL involves writing the values of \( x \) in one column and calculating the corresponding values of \( f(x) \) until it is sufficiently close to zero.

<table>
<thead>
<tr>
<th>( x )</th>
<th>( f(x) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.0</td>
<td>-2.0403023</td>
</tr>
<tr>
<td>1.1</td>
<td>-1.6225961</td>
</tr>
<tr>
<td>1.2</td>
<td>-1.1343578</td>
</tr>
<tr>
<td>1.3</td>
<td>-0.5704988</td>
</tr>
<tr>
<td>1.4</td>
<td>0.0740329</td>
</tr>
</tbody>
</table>

From the table above, it is clear that the equation has a solution between 1.3 and 1.4 (closer to 1.4). Therefore, further iterations may lead to the following

<table>
<thead>
<tr>
<th>( x )</th>
<th>( f(x) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.38</td>
<td>-0.0615688</td>
</tr>
<tr>
<td>1.39</td>
<td>0.0058060</td>
</tr>
</tbody>
</table>

Thus, a solution between 1.38 and 1.39 (closer to 1.39) may be sought. Eventually, trial and error can establish 1.3891432 as a sufficiently accurate solution. This method is guaranteed to converge.

Iteration Method

This method arranges the nonlinear equation in a manner as to separate \( x \) on one side and a function \( g(x) \) on the other, so that successive values of \( x \) results in values of \( g(x) \), which can be used as \( x \) for the next iteration until a solution is reached.

For example, \( x^3 - \cos(x) - 2.5 = 0 \) can be rearranged as \( x = (\cos(x) + 2.5)^{1/3} = g(x) \)

<table>
<thead>
<tr>
<th>( x )</th>
<th>( g(x) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.0</td>
<td>1.4486793</td>
</tr>
<tr>
<td>1.4486793</td>
<td>1.3789037</td>
</tr>
<tr>
<td>1.3789037</td>
<td>1.3908790</td>
</tr>
<tr>
<td>1.3908790</td>
<td>1.3888482</td>
</tr>
</tbody>
</table>

It is clear that \( x \) is converging to the exact value. However, this method does not guarantee a converged solution; e.g., \( x = \cos^{-1}(x^3 - 2.5) \) doesn’t converge even with an initial guess of \( x=1.39 \).
Bisection Method

The basic principle of this method is the theorem that ‘If \( f(x) \) is continuous in an interval \( x_1 \leq x_3 \leq x_2 \) and if \( f(x_1) \) and \( f(x_2) \) are of opposite signs, then \( f(x_3) = 0 \) for at least one number \( x_3 \) such that \( x_1 < x_3 < x_2 \)’. This method is implemented using the following steps:

1. Assume two values of \( x \) (i.e., \( x_1 \) and \( x_2 \)) such that \( f(x_1) \) and \( f(x_2) \) are of opposite signs.
2. Calculate \( x_3 = (x_1 + x_2)/2 \) and \( y_3 = f(x_3) \).
3. (i) Replace \( x_1 \) by \( x_3 \) if \( f(x_1) \) and \( f(x_3) \) are of the same sign or
   (ii) Replace \( x_2 \) by \( x_3 \) if \( f(x_2) \) and \( f(x_3) \) are of the same sign.
4. Return to Step 2 and carry out the same calculations, until the difference between successive approximations is less than the allowable limit, \( \epsilon \).

Calculations for the example mentioned before can be carried out in the following manner:

<table>
<thead>
<tr>
<th>( x )</th>
<th>( f(x) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.000000</td>
<td>-2.0403023</td>
</tr>
<tr>
<td>2.000000</td>
<td>5.9161468</td>
</tr>
<tr>
<td>1.500000</td>
<td>0.8042628</td>
</tr>
<tr>
<td>1.250000</td>
<td>-0.8621974</td>
</tr>
<tr>
<td>1.375000</td>
<td>-0.0949383</td>
</tr>
<tr>
<td>1.437500</td>
<td>0.3375570</td>
</tr>
<tr>
<td>1.406250</td>
<td>0.1171095</td>
</tr>
<tr>
<td>1.390625</td>
<td>0.0100452</td>
</tr>
</tbody>
</table>

The method is guaranteed to converge provided a solution does exist. The number of steps required for convergence will depend on the interval \( (x_2 - x_1) \) and the tolerance \( (\epsilon) \). A FORTRAN program implementing the algorithm involved in this method is shown below.

```fortran
READ*,X1,X2,EPS
N=LOG(ABS(X2-X1)/EPS)/LOG(2.)
Y1=FUN(X1)
Y2=FUN(X2)
IF(Y1*Y2.GE.0)THEN
  PRINT*,X1,Y1,X2,Y2
  GOTO 11
ENDIF
DO I=1,N
  X3=(X1+X2)/2.
  Y3=FUN(X3)
  IF(ABS(X1-X2)/2.LT.EPS)GOTO 10
  IF(FUN(X1)*Y3.GT.0)X1=X3
  IF(FUN(X2)*Y3.GT.0)X2=X3
ENDDO
10 PRINT*,X3,Y3,I
11 END
FUNCTION FUN(X)
  FUN=X**3-COS(X)-2.5
END
```
Secant Method

Like the Bisection Method, the Secant Method also needs two assumed solutions of the given equation to start with. However unlike the Bisection Method it does not proceed by successively bisecting the range of solutions but rather by linear interpolation/extrapolation between assumed values.

\[
\text{Slope} = \frac{f(x_2) - f(x_1)}{x_2 - x_1} = \frac{f(x_2)}{x_2 - x_3}
\]

This method is implemented using the following steps

1. Assume two values of x (i.e., \(x_1\) and \(x_2\)) and calculate \(f(x_1)\) and \(f(x_2)\)
2. Calculate \(x_3 = x_2 - \frac{f(x_2)(x_2 - x_1)}{f(x_2) - f(x_1)}\)
3. Return to Step 2 and carry out the same calculations, replacing \(x_1\) and \(x_2\) by \(x_2\) and \(x_3\) until the difference between successive approximations is less than the allowable limit, \(\varepsilon\).

Calculations for the example mentioned before can be carried out in the following manner. If \(x_1\) and \(x_2\) are 1.0 and 1.2 respectively, both \(f(x_1)\) and \(f(x_2)\) are positive and the following calculations result.

<table>
<thead>
<tr>
<th>(x)</th>
<th>(f(x))</th>
<th>(x_3)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.0000000</td>
<td>−2.0403023</td>
<td>**********</td>
</tr>
<tr>
<td>1.2000000</td>
<td>−1.1343578</td>
<td>1.4504254 [(x_1 = 1.0000000, x_2 = 1.2000000)]</td>
</tr>
<tr>
<td>1.4504254</td>
<td>0.4312287</td>
<td>1.3814477 [(x_1 = 1.2000000, x_2 = 1.4504254)]</td>
</tr>
<tr>
<td>1.3814477</td>
<td>−0.0518677</td>
<td>1.3888535 [(x_1 = 1.4504254, x_2 = 1.3814477)]</td>
</tr>
<tr>
<td>1.3888535</td>
<td>−0.0019618</td>
<td>1.3891446 [(x_1 = 1.3814477, x_2 = 1.3888535)]</td>
</tr>
<tr>
<td>1.3891446</td>
<td>0.00000095</td>
<td>1.3891432 [(x_1 = 1.3888535, x_2 = 1.3891446)]</td>
</tr>
<tr>
<td>1.3891432</td>
<td>0.00000000</td>
<td>1.3891432 [(x_1 = 1.3891446, x_2 = 1.3891432)]</td>
</tr>
</tbody>
</table>

But if \(x_1\) and \(x_2\) are 1.0 and 2.0 respectively, \(f(x_1)\) and \(f(x_2)\) have opposite signs. One variation of the Secant Method (Regula Falsi Method) requires \(f(x_1)\) and \(f(x_2)\) to have opposite signs at each iteration.

<table>
<thead>
<tr>
<th>(x)</th>
<th>(f(x))</th>
<th>(x_3)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.0000000</td>
<td>−2.0403023</td>
<td>**********</td>
</tr>
<tr>
<td>2.0000000</td>
<td>5.9161468</td>
<td>1.2564338 [(x_1 = 1.0000000, x_2 = 2.0000000)]</td>
</tr>
<tr>
<td>1.2564338</td>
<td>−0.8257715</td>
<td>1.3475081 [(x_1 = 1.2564338, x_2 = 2.0000000)]</td>
</tr>
<tr>
<td>1.3475081</td>
<td>−0.2746616</td>
<td>1.3764566 [(x_1 = 1.3475081, x_2 = 2.0000000)]</td>
</tr>
<tr>
<td>1.3764566</td>
<td>−0.0852390</td>
<td>1.3853129 [(x_1 = 1.3764566, x_2 = 2.0000000)]</td>
</tr>
<tr>
<td>1.3853129</td>
<td>−0.0258789</td>
<td>1.3879900 [(x_1 = 1.3853129, x_2 = 2.0000000)]</td>
</tr>
<tr>
<td>1.3879900</td>
<td>−0.0078044</td>
<td>1.3887963 [(x_1 = 1.3879900, x_2 = 2.0000000)]</td>
</tr>
<tr>
<td>1.3887963</td>
<td>−0.0023489</td>
<td>1.3890389 [(x_1 = 1.3887963, x_2 = 2.0000000)]</td>
</tr>
</tbody>
</table>

The Secant Method is guaranteed to converge and convergence is faster than the Bisection Method.
Newton-Raphson (Tangent) Method

Instead of linear interpolation/extrapolation between two points by a chord as done in the Secant Method, the Newton-Raphson Method proceeds through tangents of successive approximations. Only one assumed solution of the given equation is needed to start the process. If \( x_2 \) is to be the solution of the nonlinear equation \( f(x) = 0 \) and \( x_1 \) is the first estimate, then \( f(x_2) = 0 \). Therefore Taylor’s series yields:

\[
f(x_2) = f(x_1) + (x_2-x_1) f'(x_1) + \frac{(x_2-x_1)^2}{2!} f''(x_1) + \ldots
\]

\[
0 \equiv f(x_1) + (x_2-x_1) f'(x_1) \Rightarrow x_2 = x_1 - \frac{f(x_1)}{f'(x_1)}
\]

Therefore, the Newton-Raphson Method requires only one initial guess. However, it also requires the first differentiation \( f'(x_1) \) of the function \( f(x_1) \).

Calculations for the example mentioned before \([f(x) = x^3 - \cos(x) - 2.5 = 0]\) can be carried out in the following manner, assuming \( x_1 \) to be 1.0. Therefore, \( f'(x) = 3x^2 + \sin(x) \)

<table>
<thead>
<tr>
<th>( x_1 )</th>
<th>( f(x_1) )</th>
<th>( f'(x_1) )</th>
<th>( x_2 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.000000</td>
<td>-2.0403023</td>
<td>3.841471</td>
<td>1.5311253</td>
</tr>
<tr>
<td>1.531125</td>
<td>1.0498246</td>
<td>8.032247</td>
<td>1.4004240</td>
</tr>
<tr>
<td>1.400424</td>
<td>0.0769448</td>
<td>6.869084</td>
<td>1.3892224</td>
</tr>
<tr>
<td>1.389222</td>
<td>0.0005366</td>
<td>6.773378</td>
<td>1.3891432</td>
</tr>
<tr>
<td>1.389143</td>
<td>0.0000000</td>
<td>6.772703</td>
<td>1.3891432</td>
</tr>
</tbody>
</table>

The Newton-Raphson method does not guarantee converged correct solution in all situations. The convergence of this method depends on the nature of the function \( f(x) \) and the initial guess \( x_1 \). With \( f'(x) \) being the denominator on the right side of the main equation, the solution may diverge or converge to a wrong solution or continue to oscillate within a range if the slope \( f'(x) \) of the function tends to zero in the vicinity of the solution; i.e., if \( f'(x) = 0 \) anywhere between the initial guess \( x_1 \) and the actual solution.
Solution of Simultaneous Linear Equations

It is common in many engineering (also Civil Engineering in particular) applications to encounter problems involving the solution of a set of simultaneous linear equations. Their Civil Engineering applications include curve fitting, structural analysis, mix design, pipe-flow, hydrologic problems, etc.

Simultaneous equations can be solved by direct or indirect methods. The direct methods lead to the direct solution without making any prior assumption. The indirect solution schemes usually involve initial guesses and successive iterations until convergence to a value sufficiently close to the exact result.

Problem Formulation

A set of N linear equations can be written in the general form:

\[ A_{11} x_1 + A_{12} x_2 + \ldots + A_{1N} x_N = b_1 \]

\[ A_{21} x_1 + A_{22} x_2 + \ldots + A_{2N} x_N = b_2 \]

\[ \vdots \]

\[ A_{N1} x_1 + A_{N2} x_2 + \ldots + A_{NN} x_N = b_N \]

This can be written as \([A]{x} = {b}\), where \([A]\) is a \((N \times N)\) matrix, \({x}\) and \({b}\) are \((N \times 1)\) vectors.

Solution of Two Simultaneous Independent Linear Equations

1. Matrix Inversion

\[
\begin{bmatrix}
2 & -1 \\
3 & 4 \\
\end{bmatrix}^{-1} = \begin{bmatrix}
4 & -3 \\
1 & 2 \\
\end{bmatrix}
\]

\[
\begin{bmatrix}
x_1 \\
x_2 \\
\end{bmatrix} = \begin{bmatrix}
4 & -3 \\
1 & 2 \\
\end{bmatrix}^{-1} \begin{bmatrix}
1 \\
-5 \\
\end{bmatrix} = \begin{bmatrix}
4/11 & 1/11 \\
-3/11 & 2/11 \\
\end{bmatrix} \begin{bmatrix}
1 \\
-2 \\
\end{bmatrix}
\]

2. Cramer’s Rule

\[ x_1 = \frac{4 \times (-5) - 4 \times 3}{2 \times 4 - (-1) \times 3} = \frac{-22}{11} = -2 \]

\[ x_2 = \frac{2 \times (-5) - 4 \times 3}{2 \times 4 - (-1) \times 3} = \frac{-11}{5.5} = -2 \]

3. Gauss Elimination

\[
\begin{bmatrix}
2 & -1 \\
3 & 4 \\
\end{bmatrix} \begin{bmatrix}
x_1 \\
x_2 \\
\end{bmatrix} = \begin{bmatrix}
4 \\
-5 \\
\end{bmatrix} \Rightarrow \begin{bmatrix}
2 & -1 \\
3 & (3/2)2 \\
\end{bmatrix} \begin{bmatrix}
x_1 \\
x_2 \\
\end{bmatrix} = \begin{bmatrix}
4 \\
-11 \\
\end{bmatrix}
\]

\[ r_2' = r_2 - (3/2) r_1 \]

\[ x_2 = -11/5.5 = -2, \quad x_1 = (4 + x_2)/2 = 2/2 = 1 \]

4. Gauss-Jordan Elimination

\[
\begin{bmatrix}
2 & -1 \\
3 & 4 \\
\end{bmatrix} \begin{bmatrix}
x_1 \\
x_2 \\
\end{bmatrix} = \begin{bmatrix}
4 \\
-5 \\
\end{bmatrix} \Rightarrow \begin{bmatrix}
2 & -1 \\
0 & 5.5 \\
\end{bmatrix} \begin{bmatrix}
x_1 \\
x_2 \\
\end{bmatrix} = \begin{bmatrix}
4 \\
-11 \\
\end{bmatrix} \Rightarrow \begin{bmatrix}
2 & 0 \\
0 & 5.5 \\
\end{bmatrix} \begin{bmatrix}
x_1 \\
x_2 \\
\end{bmatrix} = \begin{bmatrix}
2 \\
-11 \\
\end{bmatrix}
\]

\[ r_1' = r_1 - (4 \times 5.5) r_2 \]

\[ x_2 = -11/5.5 = -2, \quad x_1 = 2/2 = 1 \]
Solution of Three Simultaneous Linear Equations

\[
\begin{align*}
2x_1 - x_2 - x_3 &= 5 \\
3x_1 + 4x_2 &= -5 \\
x_1 - 5x_3 &= 6
\end{align*}
\]

\[
\begin{pmatrix}
2 & -1 & -1 & 5 \\
3 & 4 & 0 & -5 \\
1 & 0 & -5 & 6
\end{pmatrix}
\implies
\begin{pmatrix}
2 & -1 & -1 & 5 \\
0 & 5.5 & 1.5 & -12.5 \\
0 & 0.5 & -4.5 & 3.5
\end{pmatrix}
\]

1. Gauss Elimination

\[r_2' = r_2 - (3/2) r_1\]

\[x_3 = 4.64 / (-4.64) = -1\]

\[r_3' = r_3 - (1/2) r_1\]

\[x_2 = (-12.5 - 1.5 \times (-1)) / 5.5 = -2\]

\[r_3'' = r_3' - (0.5/5.5) r_2'\]

\[x_1 = (5 + 1 \times (-1) + 1 \times (-2)) / 2 = 1\]

2. Gauss-Jordan Elimination

\[r_2'' = r_2' - (1/2) r_1\]

\[r_3''' = r_3'' - (0.5/5.5) r_2''\]

\[x_3 = 2/2 = 1, x_2 = -11 / 5.5 = -2, x_3 = 4.64 / (-4.64) = -1\]
Practice Problems on Simultaneous Linear Equations

1. If materials A and B are mixed at a 1:3 ratio, the density of the mixture becomes 2.15 gm/cc. If the density of B is 1.00 gm/cc more than the density of A, calculate the density of A and B using the Matrix Inversion method.

2. The axial capacity of a 160 in\(^2\) column of steel ratio 2\% (i.e., steel area/gross area = 0.02) is 500 kips. A 120 in\(^2\) column can obtain the same axial capacity if the steel ratio is increased to 5\%. Using Cramer’s Rule calculate the axial strength (axial capacity per unit area) of concrete and steel.

3. A student takes three courses (Surveying, Math and Drawing) of credit hours 4, 3 and 1.5 respectively in a summer semester. He gets equal scores in Surveying and Math and scores 80\% in Drawing. If his average semester grade in 70\%, calculate the scores in all the subjects using Gauss-Jordan Method.

4. In an essay competition, the first prize was worth Tk. 2000 comprising of three books, two pens and a crest, the second prize was worth Tk. 1500 comprising of a book, two pens and a crest while the third prize was worth Tk. 1000 comprising of a book, a pen and a crest. Using Gauss Elimination, calculate the cost of each book, pen and crest.

5. The costs of concrete mixes (by volume) at the ratios 1:3:6, 1:2:4 and 1:2:3 are 200, 225 and 240 Taka/ft\(^2\) respectively. Calculate the cost per ft\(^2\) of cement, sand and coarse aggregate using Gauss Elimination.
General Algorithm for Gauss Elimination

1. Triangularization:

The first task of Gauss Elimination is to transform the coefficient matrix \( A \) to an upper triangular matrix. This is performed as shown below.

\[
\begin{pmatrix}
A_{11} & A_{12} & A_{13} & \ldots & A_{1N} & B_1 \\
A_{21} & A_{22} & A_{23} & \ldots & A_{2N} & B_2 \\
A_{31} & A_{32} & A_{33} & \ldots & A_{3N} & B_3 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
A_{N1} & A_{N2} & A_{N3} & \ldots & A_{NN} & B_N
\end{pmatrix}
\]

\[
\begin{pmatrix}
A_{11} & A_{12} & A_{13} & \ldots & A_{1N} & B_1 \\
0 & A_{22} - r_{21} (A_{12}) & A_{23} - r_{21} (A_{13}) & \ldots & A_{2N} - r_{21} (A_{1N}) & B_2 - r_{21} (B_1) \\
0 & A_{32} - r_{31} (A_{12}) & A_{33} - r_{31} (A_{13}) & \ldots & A_{3N} - r_{31} (A_{1N}) & B_3 - r_{31} (B_1) \\
0 & A_{42} - r_{41} (A_{12}) & A_{43} - r_{41} (A_{13}) & \ldots & A_{4N} - r_{41} (A_{1N}) & B_4 - r_{41} (B_1) \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
0 & A_{N2} - r_{N1} (A_{12}) & A_{N3} - r_{N1} (A_{13}) & \ldots & A_{NN} - r_{N1} (A_{1N}) & B_N - r_{N1} (B_1)
\end{pmatrix}
\]

\[
\begin{pmatrix}
A_{11} & A_{12} & A_{13} & \ldots & A_{1N} & B_1 \\
0 & 0 & A_{33} - r_{32} (A_{23}) & \ldots & A_{3N} - r_{32} (A_{2N}) & B_1' - r_{21} (B_1) \\
0 & 0 & A_{43} - r_{42} (A_{23}) & \ldots & A_{4N} - r_{42} (A_{2N}) & B_1' - r_{21} (B_1) \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & A_{N3} - r_{N2} (A_{2N}) & \ldots & A_{NN} - r_{N2} (A_{2N}) & B_1' - r_{21} (B_1)
\end{pmatrix}
\]

and so on.

\[\therefore \text{In general, } A_{ij}^{(k)} = A_{ij}^{(k-1)} - r_{ik}^{(k-1)} (A_{kj})^{(k-1)} \text{ and } B_i^{(k)} = B_i^{(k-1)} - r_{ik}^{(k-1)} (B_k)^{k-1}\]

where \( r_{ik}^{(k-1)} = A_{ik}^{(k-1)} / A_{kk}^{(k-1)} \). Here \( k \) varies between \( 1 \sim (N-1) \), while \( i \) and \( j \) vary between \( (k+1) \sim N \).

2. Back Substitution:

Once the matrix \( A \) is transformed to an upper triangular matrix, the unknowns can be calculated by Back Substitution. This is performed as follows.

\[ X_N = B_N / A_{NN} \]

\[ X_{N-1} = (B_{N-1} - A_{N-1,N} X_N) / A_{N-1,N} \]

\[ X_{N-2} = (B_{N-2} - A_{N-2,N-1} X_{N-1} - A_{N-2,N} X_N) / A_{N-2,N} \]

and so on.

\[ \therefore \text{In general, } X_i = (B_i - \sum A_{ik} X_k) / A_{ii} \text{ where } \sum \text{ is a summation for } k \text{ varying between } (i+1) \sim N \]. In computer programs, the vector \( \{X\} \) is rarely introduced; the unknowns are stored in the vector \( \{B\} \) itself.
FORTRAN program to implement Gauss Elimination:

```fortran
N1=N-1
DO 10 K=1,N1
   K1=K+1
   C=1./A(K,K)
   DO 11 I=K1,N
      D=A(I,K)*C
      DO 12 J=K1,N
         A(I,J)=A(I,J)–D*A(K,J)
      12
      B(I)=B(I)–D*B(K)
   11
10 CONTINUE
B(N)=B(N)/A(N,N)
DO 13 I=N1,1,-1
   I1=I+1
   SUM=0.
   DO 14 K=I1,N
      SUM=SUM+A(I,K)*B(K)
   14
   B(I)=(B(I)–SUM)/A(I,I)
13
END
```

Numerical aspects of Direct Solution of Linear Equations

1. Pivoting: A key feature in the numerical algorithm with Gauss (or Gauss-Jordan) Elimination is the triangularization (or diagonalization) of the [A] matrix. This is performed by equations like

   \[ A'_{ij} = A_{ij} - \left( A_{ik} / A_{kk} \right) (A_{kj}) \text{ and } B'_{i} = B_{i} - \left( A_{i k} / A_{kk} \right) (B_{k}) \]

   Keeping the kth row as the ‘pivot’ around which the solution hinges. Therefore if the diagonal element \( A_{kk} \) becomes zero at any stage of the computation, the solution process cannot advance further. Then it may be necessary to interchange rows (or columns) in order to get the solution. For example, the equations \( 2x_1 + 2x_2 + x_3 = 5, \ x_1 + x_2 + x_3 = 3 \) and \( 2x_1 + x_3 = 3 \) require such adjustment.

   Even if \( A_{kk} \neq 0 \), it may be necessary to interchange the rows for better accuracy. Sometimes columns are interchanged in order to use the largest element of the row as the ‘pivotal’ element.

2. Singular [A] matrix: The determinant of a singular matrix is zero; i.e., [A] is singular if \(|A| = 0\). In such cases it is not possible to obtain a solution of the set of equations because the solution vector is \( \{X\} = [A]^{-1}\{B\} \), where \([A]^{-1}\) is the inverse matrix of [A] is given by \([A]^{-1}/|A|\). Thus \( \{X\} \) is not determinate if \(|A| = 0\); e.g., the equations \( 2x_1 + x_2 = 0 \) and \( 4x_1 + 2x_2 = 5 \) have no solution.

3. Ill-conditioned [A] matrix: Even if [A] is not singular, it may pose numerical problems if \(|A| \) is ‘small’ (compared to the terms of [A]). In such cases, a small difference in [A] or \( \{B\} \) may lead to large variations in the solutions. Therefore [A], \( \{B\} \) must be known with precision and the solution must be performed accurately; e.g., solutions of \( \{100x_1 + 99x_2 = 1; 99x_1 + 98x_2 = 1\}, \{100x_1 + 99x_2 = 1; 99x_1 + 98.1x_2 = 1\} \) and \( \{100x_1 + 99x_2 = 1.1; 99x_1 + 98x_2 = 1\} \) are much different from each other.

4. Banded Matrix and Sparse Matrix: The elements of a Banded Matrix are concentrated mostly around the diagonal, while elements of a Sparse Matrix are widely spread away from the diagonal.
Iterative Methods for Solution of Simultaneous Equations

If the system of equations is diagonally dominant, iterative schemes can be used conveniently to solve them. For large systems, the computational effort needed in these methods is less than the direct solutions if a suitable initial estimate can be made. These schemes can also be used for nonlinear equations.

1. Jacobi’s Method

The general solution for this method can be written as \( x_i^{(m+1)} = \left( B_i - \sum A_{ik} x_k^{(m)} \right) / A_{ii} \) if \( A_{ii} \neq 0 \)
where \( i = 1, 2, \ldots, N \) and \( \sum \) is a summation for \( k = 1 \sim N \) (but \( k \neq i \)).

A sequence of solution vectors can be generated from \( x_i^{(m+1)} = \left( B_i - \sum A_{ik} x_k^{(m)} \right) / A_{ii} \)

For example

\[
\begin{align*}
2x_1 - x_2 - x_3 &= 5 \\
3x_1 + 4x_2 &= -5 \\
x_1 - 5x_3 &= 6
\end{align*}
\]

For \( x_1^{(m+1)} = (5 + x_2^{(m)} + x_3^{(m)})/2 \)

\( x_2^{(m+1)} = (-5 - 3x_1^{(m)})/4 \)

\( x_3^{(m+1)} = (-6 + x_1^{(m)})/5 \)

<table>
<thead>
<tr>
<th>( x_i^{(m)} )</th>
<th>( x_i^{(m+1)} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>{0.0000, 0.0000, 0.0000}</td>
<td>{2.5000, -1.2500, -1.2000}</td>
</tr>
<tr>
<td>{2.5000, -1.2500, -1.2000}</td>
<td>{1.2750, -3.1250, -0.7000}</td>
</tr>
<tr>
<td>{1.2750, -3.1250, -0.7000}</td>
<td>{0.5875, -2.2063, -0.9450}</td>
</tr>
<tr>
<td>{0.5875, -2.2063, -0.9450}</td>
<td>{0.9244, -1.6906, -1.0825}</td>
</tr>
<tr>
<td>{0.9244, -1.6906, -1.0825}</td>
<td>{1.1134, -1.9433, -1.0151}</td>
</tr>
</tbody>
</table>

2. Gauss-Seidel Method

This is a modified version of Jacobi’s Method that uses the most recently updated values of \( x_i \) in the subsequent calculations. The solution for this method for the \( m \)th and \( (m+1) \)th iterations can be written as

\( x_i^{(m+1)} = \left( B_i - \sum A_{ik} x_k^{(m+1)} - \sum A_{ik} x_k^{(m)} \right) / A_{ii} \)

where the first \( \sum \) is a summation for \( k = 1 \sim (i-1) \) and the second \( \sum \) is a summation for \( k = (i+1) \sim N \).

\[
\begin{align*}
2x_1 - x_2 - x_3 &= 5 \\
3x_1 + 4x_2 &= -5 \\
x_1 - 5x_3 &= 6
\end{align*}
\]

For \( x_1^{(m+1)} = (5 + x_2^{(m)} + x_3^{(m)})/2 \)

\( x_2^{(m+1)} = (-5 - 3x_1^{(m+1)})/4 \)

\( x_3^{(m+1)} = (-6 + x_1^{(m+1)})/5 \)

<table>
<thead>
<tr>
<th>( x_i^{(m)} )</th>
<th>( x_i^{(m+1)} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>{0.0000, 0.0000, 0.0000}</td>
<td>{2.5000, -3.1250, -0.7000}</td>
</tr>
<tr>
<td>{2.5000, -3.1250, -0.7000}</td>
<td>{0.5875, -1.6906, -1.0825}</td>
</tr>
<tr>
<td>{0.5875, -1.6906, -1.0825}</td>
<td>{1.1134, -2.0851, -0.9773}</td>
</tr>
</tbody>
</table>

The exact solution of these equations is \( x_1 = 1, x_2 = -2, x_3 = -1 \)

For nonlinear equations, direct iteration schemes like \( \{A^{(m)} \} \{X^{(m+1)} \} = \{B^{(m)} \} \) (or Newton-Raphson Method) can be used. Here, both the matrix \( A \) and vector \( B \) are functions of the solution vector \( X \).
Lagrange Interpolation

The general equation of a polynomial of n-degree is

\[ y = f(x) = a_0 + a_1 x + a_2 x^2 + \ldots + a_n x^n \]  \hspace{1cm} \text{.....(1)}

which can be rearranged as

\[ f(x) = (x-x_1)(x-x_2)\ldots(x-x_n) c_0 + (x-x_0)(x-x_2)\ldots(x-x_n) c_1 + \ldots + (x-x_0)(x-x_2)\ldots(x-x_{n-1}) c_n \]  \hspace{1cm} \text{.....(2)}

The evaluation of coefficients \( c_0, c_1, \ldots, c_n \) is much easier than the evaluation of coefficients \( a_0, a_1, \ldots, a_n \). Whereas the evaluation of coefficients \( a_0, a_1, \ldots, a_n \) needs the solution of \( n \) simultaneous equations, coefficients \( c_0, c_1, \ldots, c_n \) can be evaluated directly.

For example, putting \( x = x_0 \) in Eq. (2) \( \Rightarrow \)

\[ f(x_0) = (x_0-x_1)(x_0-x_2)\ldots(x_0-x_n) c_0 \Rightarrow c_0 = f(x_0)/(x_0-x_1)(x_0-x_2)\ldots(x_0-x_n) \]  \hspace{1cm} \text{.....(3)}

Similarly, putting \( x = x_1 \) in Eq. (2) \( \Rightarrow c_1 = f(x_1)/(x_1-x_0)(x_1-x_2)\ldots(x_1-x_n) \)  \hspace{1cm} \text{.....(4)}

Finally, putting \( x = x_n \) in Eq. (2) \( \Rightarrow c_n = f(x_n)/(x_n-x_0)(x_n-x_1)\ldots(x_n-x_{n-1}) \)  \hspace{1cm} \text{.....(5)}

Thus, all the coefficients can be evaluated directly without going through the process of simultaneous solution. Therefore, Eq. (2) can be written as

\[ f(x) = (x-x_1)(x-x_2)\ldots(x-x_n)/\{(x_0-x_1)(x_0-x_2)\ldots(x_0-x_n)\} f(x_0) + (x-x_0)(x-x_2)\ldots(x-x_n)/\{(x_1-x_0)(x_1-x_2)\ldots(x_1-x_n)\} f(x_1) + \ldots + (x-x_0)(x-x_2)\ldots(x-x_{n-1})/\{(x_n-x_0)(x_n-x_1)\ldots(x_n-x_{n-1})\} f(x_n) \]  \hspace{1cm} \text{.....(6)}

Example

Find the equation of the polynomial passing through \( (0,0), (1,2), (2,3) \) and \( (3,0) \)

Here, \( n = 3, x_0 = 0, f(x_0) = 0, x_1 = 1, f(x_1) = 2, x_2 = 2, f(x_2) = 3, x_3 = 3, f(x_3) = 0 \)

Therefore, \( f(x) = (x-1)(x-2)(x-3)/\{(0-1)(0-2)(0-3)\} 0 + (x-0)(x-2)(x-3)/\{(1-0)(1-2)(1-3)\} 2 + (x-0)(x-1)(x-3)/\{(2-0)(2-1)(2-3)\} 3 + (x-0)(x-1)(x-2)/\{(3-0)(3-1)(3-2)\} 0 \)

\[ = x (x-2)(x-3) - x (x-1)(x-3) \text{ } 3/2 \]
Newton’s Divided Difference Interpolation

Let \( y = f(x) \) be the general equation of a polynomial of \( n \)-degree that passes through points \( x_0, x_1, x_2, \ldots, x_n \).

A 1\(^{st}\) order divided difference equation for \((x, x_0)\) is given by

\[
f[x, x_0] = \left[ f(x) - f(x_0) \right]/(x - x_0) \Rightarrow f(x) = f(x_0) + (x - x_0) f[x, x_0] \quad \text{……(1)}
\]

Similarly, a 2\(^{nd}\) order divided difference equation for \((x, x_0, x_1)\) is

\[
f[x, x_0, x_1] = \left[ f[x, x_0] - f[x_0, x_1] \right]/(x - x_1) \Rightarrow f[x, x_0] = f[x_0, x_1] + (x - x_1) f[x, x_0, x_1] \quad \text{……(2)}
\]

and a 3\(^{rd}\) order equation for \((x, x_0, x_1, x_2)\) is

\[
f[x, x_0, x_1, x_2] = \left[ f[x, x_0, x_1] - f[x_0, x_1, x_2] \right]/(x - x_2) \Rightarrow f[x, x_0, x_1] = f[x_0, x_1, x_2] + (x - x_2) f[x, x_0, x_1, x_2] \quad \text{……(3)}
\]

Combining (1) and (2),

\[
f(x) = f(x_0) + (x - x_0) f[x_0, x_1] + (x - x_0) (x - x_1) f[x, x_0, x_1] \quad \text{……(4)}
\]

Therefore, the equation of a 1-degree polynomial is

\[
f(x) = f(x_0) + (x - x_0) f[x_0, x_1] \quad \text{……(5)}
\]

where \( f[x_0, x_1] = \{ f(x_0) - f(x_1) \}/(x_0 - x_1) \)

Similarly, combining (3) and (4),

\[
f(x) = f(x_0) + (x - x_0) f[x_0, x_1] + (x - x_0) (x - x_1) f[x_0, x_1, x_2] + (x - x_0) (x - x_1) (x - x_2) f[x, x_0, x_1, x_2] \quad \text{……(6)}
\]

.: Equation of a 2-degree polynomial is

\[
f(x) = f(x_0) + (x - x_0) f[x_0, x_1] + (x - x_0) (x - x_1) f[x, x_0, x_1] \quad \text{……(7)}
\]

where \( f[x_0, x_1] = \{ f(x_0) - f(x_1) \}/(x_0 - x_1) \), \( f[x_1, x_2] = \{ f(x_1) - f(x_2) \}/(x_1 - x_2) \)

and \( f[x_0, x_1, x_2] = \{ f[x_0, x_1] - f[x_1, x_2] \}/(x_0 - x_2) \)

The general equation of polynomial of \( n \)-degree is therefore

\[
f(x) = f(x_0) + (x - x_0) f[x_0, x_1] + (x - x_0) (x - x_1) f[x_0, x_1, x_2] + \ldots \ldots \ldots + (x - x_0) (x - x_1) \ldots (x - x_n-1) f[x_0, x_1, \ldots, x_n] \quad \text{……(8)}
\]

Example

Find the equation of the polynomial passing through \((0,0), (1,2), (2,3)\) and \((3,0)\)

<table>
<thead>
<tr>
<th>( x )</th>
<th>( f(x) )</th>
<th>1(^{st}) order difference</th>
<th>2(^{nd}) order difference</th>
<th>3(^{rd}) order difference</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>2</td>
<td>(2-0)/(1-0) = 2</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>3</td>
<td>(3-2)/(2-1) = 1</td>
<td>(-2+0.5)/(3-0) = -0.5</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>0</td>
<td>(-3-1)/(3-1) = -2</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

\[ f(x) = f(0) + (x-0) f[0,1] + (x-0) (x-1) f[0,1,2] + (x-0) (x-1) (x-2) f[0,1,2, 3] \]

\[ = 0 + x (2) + x (x-1) (-0.5) + x (x-1)(x-2) (-0.5) = -0.5 x^3 + x^2 +1.5 x \]
Curve Fitting using the Least-Square Method

The Principle of Least Squares

The least-square method of curve fitting is based on fitting a set of data to a particular equation so that the summation of the squares of distances between the ‘data ordinates’ and ordinates from the ‘best-fit curve’ is the minimum.

Therefore, if a set of data \((x_i, y_i)\) \([i=1\sim m]\) is fitted to an equation \(y = f(x)\), the least-square method minimizes the summation \(S = \sum(y_i - f(x_i))^2\) by adjusting the parameters of \(f(x)\).

Fitting of Straight Lines

If a set of data \((x_i, y_i)\) \([i=1\sim m]\) is to be fitted to a straight line passing through origin with an assumed equation \(y = a_1 x\), the least-square method minimizes the summation

\[ S = \sum(y_i - a_1 x_i)^2 \]  

(1)

If \(S\) is minimized, \(\frac{\partial S}{\partial a_1} = 0\) \(\Rightarrow \frac{\partial \sum(y_i - a_1 x_i)^2}{\partial a_1} = 0\) \(\Rightarrow \sum 2(y_i - a_1 x_i)(-x_i) = 0\)  

\(\Rightarrow 2\sum(-x_i y_i + a_1 x_i^2) = 0 \Rightarrow -\sum x_i y_i + a_1 \sum x_i^2 = 0\)  

(2)

\(\therefore a_1 = \frac{\sum x_i y_i}{\sum x_i^2}\)  

(3)

\(\therefore\) Once \(a_1\) is known \((= \sum x_i y_i/\sum x_i^2)\), the equation of the best-fit straight line is also known.

If the assumed equation is \(y = a_0 + a_1 x\), then summation \(S = \sum(y_i - a_0 - a_1 x_i)^2\)  

(4)

If \(S\) is minimized, \(\frac{\partial S}{\partial a_0} = 0\) \(\Rightarrow \sum 2(y_i - a_0 - a_1 x_i)(-1) = 0 \Rightarrow -\sum y_i + \sum a_0 + \sum a_1 x_i = 0\)  

\(\Rightarrow (m) a_0 + (\sum x_i) a_1 = \sum y_i\)  

(5)

also \(\frac{\partial S}{\partial a_1} = 0 \Rightarrow \sum 2(y_i - a_0 - a_1 x_i)(-x_i) = 0 \Rightarrow -\sum x_i y_i + \sum a_0 x_i + \sum a_1 x_i^2 = 0\)  

\(\Rightarrow (\sum x_i) a_0 + (\sum x_i^2) a_1 = \sum x_i y_i\)  

(6)

\(\therefore a_0\) and \(a_1\) can be calculated from Eqs. (5) and (6) and used in the equation \(y = a_0 + a_1 x\)

Example

Derive best-fit straight lines \(y = a_1 x\) and \(y = a_0 + a_1 x\) for points \((0,1), (1,2), (2,4), (3,5)\) and \((4,6)\).

(i) For the assumed equation \(y = a_1 x\), \(a_1 = \sum x_i y_i/\sum x_i^2\)

Here, \(\sum x_i^2 = 0^2+1^2+2^2+3^2+4^2 = 30\), \(\sum x_i y_i = 0\times1+1\times2+2\times4+3\times5+4\times6 = 49 \Rightarrow a_1 = 49/30 = 1.633\)

\(\therefore y = 1.633 x\) and \(S = \sum(y_i - 1.633 x_i)^2 = 1.967\)

(ii) For the assumed equation \(y = a_0 + a_1 x\)

\(m = 5\), \(\sum x_i = 0+1+2+3+4 = 10\), \(\sum x_i^2 = 30\), \(\sum y_i = 1+2+4+5+6 = 18\), \(\sum x_i y_i = 49\)

\(\Rightarrow 5 a_0 + 10 a_1 = 18; 10 a_0 + 30 a_1 = 49 \Rightarrow a_1 = 1.0, a_1 = 1.3\)

\(\therefore y = 1 + 1.3 x\) and \(S = \sum(y_i - 1 - 1.3 x_i)^2 = 0.30\)
Fitting of Polynomials

If a set of $n$ data points $(x_i, y_i)$ \[i=1,\ldots,m\] is to be fitted to a polynomial of $n$ degree with an assumed equation $y = a_0 + a_1 x + a_2 x^2 + \ldots + a_n x^n$ \hspace{1in} ..................(7)

the least-square method described before can be extended to minimize the summation

$S = \sum (y_i - a_0 - a_1 x_i - a_2 x_i^2 - \ldots - a_n x_i^n)^2$ \hspace{1in} ..................(8)

If $S$ is minimized, $\frac{\partial S}{\partial a_0} = 0 \Rightarrow \sum 2(y_i - a_0 - a_1 x_i - a_2 x_i^2 - \ldots - a_n x_i^n) (-1) = 0$

$\Rightarrow (m) a_0 + (\sum x_i) a_1 + (\sum x_i^2) a_2 + \ldots + (\sum x_i^n) a_n = \sum y_i$ \hspace{1in} ..................(9)

$\frac{\partial S}{\partial a_1} = 0 \Rightarrow (\sum x_i) a_0 + (\sum x_i^2) a_1 + (\sum x_i^3) a_2 + \ldots + (\sum x_i^{n+1}) a_n = \sum x_i y_i$ \hspace{1in} ..................(10)

$\frac{\partial S}{\partial a_n} = 0 \Rightarrow (\sum x_i^n) a_0 + (\sum x_i^{n+1}) a_1 + (\sum x_i^{n+2}) a_2 + \ldots + (\sum x_i^{2n}) a_n = \sum x_i^n y_i$ \hspace{1in} ..................(11)

: Coefficients $a_0, a_1, a_2, \ldots, a_n$ can be evaluated from the matrix equations shown below.

$$
\begin{pmatrix}
    m & \sum x_i & \sum x_i^2 & \ldots & \sum x_i^n \\
    \sum x_i & \sum x_i^2 & \sum x_i^3 & \ldots & \sum x_i^{n+1} \\
    \sum x_i^2 & \sum x_i^3 & \sum x_i^4 & \ldots & \sum x_i^{n+2} \\
    \vdots & \vdots & \vdots & \ddots & \vdots \\
    \sum x_i^n & \sum x_i^{n+1} & \sum x_i^{n+2} & \ldots & \sum x_i^{2n}
\end{pmatrix}
\begin{pmatrix}
    a_0 \\
    a_1 \\
    a_2 \\
    \vdots \\
    a_n
\end{pmatrix}
= 
\begin{pmatrix}
    \sum y_i \\
    \sum x_i y_i \\
    \sum x_i^2 y_i \\
    \vdots \\
    \sum x_i^n y_i
\end{pmatrix}
$$

Example

Derive the best-fit equation $y = a_0 + a_1 x + a_2 x^2$ for the points (0,1), (1,2), (2,4), (3,5) and (4,6).

The following summations are needed for the assumed best-fit equation $y = a_0 + a_1 x + a_2 x^2$

$m = 5, \sum x_i = 10, \sum x_i^2 = 30, \sum x_i^3 = 0+1+8+27+64 = 100, \sum x_i^4 = 0+1+16+81+256 = 354$

$\sum y_i = 18, \sum x_i y_i = 49, \sum x_i^2 y_i = 0\times 1+1^2\times 2+2^2\times 4+3^2\times 5+4^2\times 6 = 159$

$\Rightarrow 5 a_0 + 10 a_1 + 30 a_2 = 18; 10 a_0 + 30 a_1 + 100 a_2 = 49; 30 a_0 + 100 a_1 + 354 a_2 = 159$

$\Rightarrow a_0 = 0.857, a_1 = 1.586, a_2 = -0.0714$

: $y = 0.857 + 1.586 x - 0.0714 x^2$ and $S = \sum (y_i - 0.857 - 1.586 x_i + 0.0714 x_i^2)^2 = 0.2286$
Miscellaneous Best-fit Curves

1. Polynomials with Non-integer Exponents

   For example, if \( y = f(x) = a_n x^n \), where \( n \) is known and is not an integer
   
   \[
   \text{Minimization of } S = \sum (y_i - a_n x_i^n)^2 \text{ leads to } a_n = \frac{\sum x_i^n y_i}{\sum x_i^{2n}} \quad \ldots \ldots (1)
   \]

2. Polynomials with some coefficients equal to zero

   For example, if the assumed \( y = a_0 + a_3 x^3 \); i.e., \( a_1 = 0, a_2 = 0 \)
   
   \[
   \text{Minimization of } S = \sum (y_i - a_0 - a_3 x_i^3)^2 \text{ with respect to } a_0 \text{ and } a_3
   \]
   \[
   \Rightarrow (m) \quad a_0 + (\sum x_i^3) a_3 = \sum y_i \quad \ldots \ldots (4)
   \]
   \[
   \text{and } (\sum x_i^3) a_0 + (\sum x_i^6) a_3 = \sum x_i^3 y_i \quad \ldots \ldots (5)
   \]

3. Reduction of Non-linear equations to linear forms

   (i) Circle \( x^2 + y^2 = r^2 \), where \( r \) is the only unknown (to be determined from the best-fit equation).
   
   Assuming \( X = x^2 \), \( Y = y^2 \) and \( R = r^2 \) reduces the equation to \( X + Y = R \Rightarrow Y = R - X \quad \ldots \ldots (6) \)
   
   \[
   \text{Minimization of } S = \sum (Y_i - R + X_i)^2 \text{ with respect to } R
   \]
   \[
   \Rightarrow \sum Y_i = m R - \sum X_i \Rightarrow m R = \sum X_i + \sum Y_i \Rightarrow m r^2 = \sum x_i^2 + \sum y_i^2
   \]
   \[
   \Rightarrow r = \sqrt{\frac{\sum x_i^2 + \sum y_i^2}{m}} \quad \ldots \ldots (7)
   \]

(ii) \( y = f(x) = a_n x^n \), where \( a_n \) and \( n \) are the unknowns (to be determined from the best-fit equation).

   Reduction the equation to \( \log(y) = \log(a_n) + n \log(x) \quad \ldots \ldots (8) \)
   
   and assuming \( X = \log(x) \), \( Y = \log(y) \) and \( A = \log(a_n) \) reduces the equation to \( Y = A + n X \quad \ldots \ldots (9) \)
   
   \[
   \text{Minimization of } S = \sum (Y_i - A - n X_i)^2 \text{ with respect to } A \text{ and } n \text{ leads to}
   \]
   \[
   \Rightarrow (m) \quad A + (\sum X_i) n = \sum Y_i \quad \ldots \ldots (10)
   \]
   \[
   \text{and } (\sum X_i) A + (\sum X_i^2) n = \sum X_i Y_i \quad \ldots \ldots (11)
   \]
   
   Once \( A \) and \( n \) are determined from Eqs. (10) and (11), \( a_n = e^A \) is also known and is used in the equation \( y = f(x) = a_n x^n \).

(iii) \( y = a_0 + a_1/x \)

   \[
   \text{Minimization of } S = \sum (y_i - a_0 - a_1/x_i)^2 \text{ with respect to } a_0 \text{ and } a_1
   \]
   \[
   \Rightarrow (m) \quad a_0 + (\sum 1/x_i) a_1 = \sum y_i \quad \ldots \ldots (13)
   \]
   \[
   \text{and } (\sum 1/x_i) a_0 + (\sum 1/x_i^2) a_1 = \sum y_i/x_i \quad \ldots \ldots (14)
   \]

(iv) \( y = 1 - e^{-b x} \) where \( b \) is the only unknown (to be determined from the best-fit equation).

   Reducing the equation to \( \log(1-y) = -b x \quad \ldots \ldots (15) \)
   
   and assuming \( Y = \log(1-y) \) reduces the equation to \( Y = -b x \quad \ldots \ldots (16) \)
   
   \[
   \text{Minimization of } S = \sum (Y_i + b x)^2 \text{ with respect to } b \Rightarrow b = -\sum (x_i Y_i)/(\sum x_i^2) \quad \ldots \ldots (17)
   \]
Practice Problems on Interpolation and Curve Fitting

1. Given the (x,y) ordinates of six points (0,2.2) , (0.9,2.5) , (2.1,3.1) , (3.2,3.5) , (3.9,3.9) , (4.6,5.0), fit
   (i) a straight line through origin \[ y = f(x) = a_1 x \], (ii) a general straight line \[ y = f(x) = a_0 + a_1 x \],
   (iii) a parabola \[ y = f(x) = a_0 + a_2 x^2 \] and (iv) a general parabola \[ y = f(x) = a_0 + a_1 x + a_2 x^2 \] through
   this set of data points. Calculate \( S \) and \( f(2.5) \) in each case.

2. Use Newton’s and Lagrange’s interpolation scheme to fit a general polynomial \( (n = 5) \)
   \[ y = f(x) = a_0 + a_1 x +….+ a_5 x^5 \] through the data points mentioned in Problem 1. Calculate \( f(2.5) \) in this case.

3. The discharge (Q) through a hydraulic structure for different values of head (H) is shown in Table–1.
   Calculate the discharge Q for H = 3.0 ft, using Newton’s Divided-Difference Interpolation Method.

   \[
   \begin{array}{|c|c|c|c|c|}
   \hline
   H (ft) & 1.2 & 2.1 & 2.7 & 4.0 \\
   Q (cft/sec) & 25 & 60 & 90 & 155 \\
   \hline
   \end{array}
   \]

4. Using the least-square method, fit an equation of the form \( Q = 20 H^n \) for the data shown in Table–1
   (i) using the polynomial form (ii) using \( \log (Q/20) = n \log (H) \); i.e., \( Y = nX \).
   In each case, calculate the discharge Q for H = 3.0 ft.

5. Using the least-square method, fit an equation of the form \( Q = K H^n \) [i.e., \( \log Q = \log K + n \log (H) \)]
   for the data shown in Table–1. Using the best-fit equation, calculate the discharge Q for H = 3.0 ft.

6. Table–2 shows the deflection (\( \delta \)) of a cantilever beam at different distances (x) from one end.
   Calculate \( \delta \) for x = 10 ft using Newton’s Divided-Difference Interpolation Method.

   \[
   \begin{array}{|c|c|c|c|c|}
   \hline
   x (ft) & 3 & 6 & 9 & 12 \\
   \delta (mm) & 3 & 11 & 22 & 35 \\
   \hline
   \end{array}
   \]

7. Use the least-square method to fit an equation of the form \( \delta = ax^n \) for the data shown in Table–2.
   Using the best-fit equation, calculate \( \delta \) for x = 10 ft.

8. Derive a best-fit equation of the form \( \delta = a (1–\cos \pi x/24) \) for the data shown in Table–2 and calculate
   \( \delta \) for x = 10 ft using the best-fit equation.

9. The strength (S) of concrete at different times (t) is shown in Table–3. Calculate the strength S for t =
   28 days, using Lagrange Interpolation Method.

   \[
   \begin{array}{|c|c|c|c|c|}
   \hline
   t (days) & 3 & 7 & 14 & 21 \\
   S (ksi) & 1.3 & 1.8 & 2.3 & 2.5 \\
   \hline
   \end{array}
   \]

10. Use the least-square method to fit an equation of the form \( S = at^{0.5} \) for the data shown in Table–3.
    Using the best-fit equation, calculate S for t = 28 days.

11. Derive a best-fit equation of the form \( S = 3(1–e^{-at}) \) [i.e., \( \log_e(1–S/3) = –at \)] for the data shown in
    Table–3 and calculate S for t = 28 days using the best-fit equation.
Numerical Differentiation

Differentiation of Interpolated Polynomial

Given a set of data points \((x_i, y_i)\) \([i=0–m]\), a general polynomial (of \(m\)-degree) can be fitted by interpolation. Once the equation of the polynomial is derived, differentiation at any point on the curve can be carried out as many times as desired.

For example, the equation of the polynomial passing through \((0,0)\), \((1,2)\), \((2,3)\) and \((3,0)\) is

\[
y = f(x) = -0.5 \times^3 + x^2 + 1.5 \times
\]

Therefore, \(dy/dx = f'(x) = -1.5 \times^2 + 2 \times + 1.5\), \(d^2y/dx^2 = f''(x) = -3 \times + 2, d^3y/dx^3 = f'''(x) = -3\)

\[
\therefore f'(0) = 1.5, f'(1) = 2, f'(2) = -0.5, f'(3) = -6; \text{ also, } f'(-1.5) = 4.875, f'(1.5) = 1.125, f'(4.0) = -14.5
\]

\[
f'''(1) = -1, f'''(1.5) = -2.5, f'''(2) = -4, f'''(2) = -3
\]

The advantage of this method is that once the equation of the polynomial is obtained, differentiations at any point (not only the data points) can be performed easily. However, the interpolation schemes may require more computational effort than is necessary for differentiation at one point or only a few specific points. Moreover, this method cannot be used for cases when the equation of the curve is not known.

The Finite Difference Method

Assuming simplified polynomial equations between points of interest, differentiations are written in discretized forms; e.g.,

at point B in Fig. 1

\[
y' = dy/dx = (y_2 - y_0)/2h \quad \text{………………(1)}
\]

\[
y'' = d^2y/dx^2 = (y_2 - 2y_1 + y_0)/h^2 \quad \text{………………(2)}
\]

Higher order differentiations can be defined similarly.

Equations (1) and (2) above are called ‘Central Difference Formulae’ because they involve the points on the left and right of the point of interest (i.e., point B in this case).

Differentiations can also be defined in terms of points on the right or on the left of the point of interest, the formulae being called the ‘Forward Difference Formulae’ and the ‘Backward Difference Formulae’ respectively. For example, the ‘Forward Difference Formula’ for \(y'(=dy/dx)\) at B is

\[
y'_{(+)} = (y_2 - y_1)/h \quad \text{……………………(3)}
\]

while the ‘Backward Difference Formula’ is \(y'_{(-)} = (y_1 - y_0)/h \quad \text{……………………(4)}\)

Despite several limitations, this method is used often in numerical solution of differential equations.

For example, for the given points \((0,0)\), \((1,2)\), \((2,3)\) and \((3,0)\)

Using Central Difference, \(f'(1) = (3-0)/(2\times1) = 1.5, f'(2) = (0-2)/(2\times1) = -1\)

\(f''(1) = (3-2\times2+0)/(1)^2 = -1, f''(2) = (0-2\times3+2)/(1)^2 = -4\)

Forward Diff. \(\Rightarrow f'(1) = (3-2)/1 = 1, f'(0) = 2, \text{ Backward Diff. } \Rightarrow f'(1) = (2-0)/1 = 2, f'(3) = -3\)
Numerical Integration

1. Trapezoidal Rule:

   In this method, the area is divided into n trapeziums, connected by straight lines between (n+1) ordinates.

   Area of the 1st trapezium, \( A_1 = h \left( y_0 + y_1 \right)/2 \)

   Area of the 2nd trapezium, \( A_2 = h \left( y_1 + y_2 \right)/2 \)

   .................................................................

   Area of the n\(^{th}\) trapezium, \( A_n = h \left( y_{n-1} + y_n \right)/2 \)

   \[ \therefore \text{Total area, } A = A_1 + A_2 + \ldots + A_n = h \left\{ \left( y_0 + y_n \right)/2 + \left( y_1 + y_2 + \ldots + y_{n-1} \right) \right\} \] \hspace{1cm} \text{..................(1)}

2. Simpson’s Rule:

   In this method, the area is divided into n/2 parabolas, each obtained by interpolating between three points. Using Lagrange’s interpolation, the equation of a parabola between points \((-h, y_0), (0, y_1), \text{ and } (h, y_2)\) is given by

   \[ y = \left\{ \frac{(x-0)(x-h)/(-h)(-2h)}{y_0} + \frac{(x+h)(x-h)/(h)(-h)}{y_1} + \frac{(x+h)(x-0)/(2h)(h)}{y_2} \right\} \]

   \[ = \left\{ \frac{x(x-h)(2h^2)}{y_0} + \frac{(h^2-x^2)(h^2)}{y_1} + \frac{x(x+h)(2h^2)}{y_2} \right\} \]

   Evaluating \( \int y \, dx \) between \(-h\) and \(h\), area under the curve is

   \[ A_1 = h \left( y_0 + 4y_1 + y_2 \right)/3 \]

   Similarly \( A_2 = h \left( y_2 + 4y_3 + y_4 \right)/3, A_3 = h \left( y_4 + 4y_5 + y_6 \right)/3, \ldots \ldots \ldots \ldots A_{n/2} = h \left( y_{n-2} + 4y_{n-1} + y_n \right)/3 \)

   \[ \therefore \text{Total area, } A = A_1 + A_2 + \ldots + A_{n/2} \]

   \[ = \left( h/3 \right) \left\{ y_0 + y_n + 4 \left( y_1 + y_3 + \ldots + y_{n-1} \right) + 2 \left( y_2 + y_4 + \ldots + y_{n-2} \right) \right\} \] \hspace{1cm} \text{...............(2)}

3. Gaussian Integration:

   In this method, the basic integrations are carried out between \(-1\) and \(+1\); i.e.,

   \[ \int f(\xi) \, d\xi = \sum A_i f(\xi_i) = A_1 f(\xi_1) + A_2 f(\xi_2) + A_3 f(\xi_3) + \ldots + A_n f(\xi_n) \]

   \[ \hspace{1cm} \text{.........................................................(3)} \]

   1\(^{\circ}\) polynomial, \( f(\xi) = a_0 + a_1 \xi \Rightarrow \int f(\xi) \, d\xi = 2a_0 \) + 0, which is represented by

   \[ A_1 f(\xi_1) = A_1 \left( a_0 + a_1 \xi_1 \right), \text{ where } [a_0] \Rightarrow A_1 = 2, [a_1] \Rightarrow \xi_1 = 0; \text{ this is exact up to } 1^\circ \text{ polynomial.} \]

   3\(^{\circ}\) polynomial, \( f(\xi) = a_0 + a_1 \xi + a_2 \xi^2 + a_3 \xi^3 \Rightarrow \int f(\xi) \, d\xi = 2a_0 + 0 + (2/3) a_2 + 0, \) which is represented by

   \[ A_1 f(\xi_1) + A_2 f(\xi_2) = A_1 \left( a_0 + a_1 \xi_1 + a_2 \xi_1^2 + a_3 \xi_1^3 \right) + A_2 \left( a_0 + a_1 \xi_2 + a_2 \xi_2^2 + a_3 \xi_2^3 \right), \text{ where} \]

   \[ [a_0] \Rightarrow A_1 + A_2 = 2, [a_1] \Rightarrow A_1 \xi_1 + A_2 \xi_2 = 0, [a_2] \Rightarrow A_1 \xi_1^2 + A_2 \xi_2^2 = 2/3, [a_3] \Rightarrow A_1 \xi_1^3 + A_2 \xi_2^3 = 0 \]

   Solving, \( A_1 = 1, A_2 = 1, \xi_1 = 1/\sqrt{3}, \xi_2 = -1/\sqrt{3}; \text{ this is exact up to } 3^\circ \text{ polynomial.} \]

   Similar values can be evaluated for higher order polynomials. In general, the n-point formula is exact up to \((2n-1)^\circ\) polynomial. Once integrated between \(-1\) and \(+1\), functions can be integrated between any other limits ‘a’ and ‘b’ by coordinate transformation.
Area, Centroid and Moment of Inertia using Numerical Integration

Calculate the area (A), centroidal x and y coordinates (\( \bar{x} \) and \( \bar{y} \)) and moments of inertia (I_y and I_x) about x and y axes for the shaded area shown in Fig. 1.

Exact Integration:
The exact results calculated by integration are the following (where all the \( \int \) signs indicate integration between \( x = 1 \) and \( x = 2 \)).

\[
\text{Area, } A = \int (e^{x} - 1) \, dx = (e^2 - 2) - (e^1 - 1) = 3.671
\]
\[
\bar{x} A = \int x \cdot (e^{x} - 1) \, dx = 5.889
\Rightarrow \bar{x} = 1.604
\]
\[
\bar{y} A = \int (e^{2x} - 1)/2 \, dx = 11.302
\Rightarrow \bar{y} = 3.079
\]
\[
I_y = \int x^2 \cdot (e^{x} - 1) \, dx = 9.727 \Rightarrow r_y = \sqrt{(I_y/A)} = 1.628
\]
\[
I_x = \int (e^{3x} - 1)/3 \, dx = 42.260 \Rightarrow r_x = \sqrt{(I_x/A)} = 3.393
\]

Fig. 1

Trapezoidal Rule (n = 2):
\[
\text{Area, } A = 0.5 \times \left\{ (e^1 - 1) + (e^2 - 1) \right\}/2 + (e^{1.5} - 1) = 3.768
\]
\[
\bar{x} A = 0.5 \times \left\{ 1 \times (e^1 - 1) + 2 \times (e^2 - 1) \right\}/2 + 1.5 \times (e^{1.5} - 1) = 6.235 \Rightarrow \bar{x} = 1.655
\]
\[
\bar{y} A = 0.5 \times \left\{ (e^2 - 1) + (e^1 - 1) \right\}/2 + (e^3 - 1)/2 = 12.270 \Rightarrow \bar{y} = 3.257
\]
\[
I_y = 0.5 \times \left\{ 1^2 \times (e^1 - 1) + 2^2 \times (e^2 - 1) \right\}/2 + 1.5^2 \times (e^{1.5} - 1) = 10.736 \Rightarrow r_y = \sqrt{(I_y/A)} = 1.688
\]
\[
I_x = 0.5 \times \left\{ (e^3 - 1) + (e^6 - 1) \right\}/2 + (e^{4.5} - 1)/3 = 49.962 \Rightarrow r_x = \sqrt{(I_x/A)} = 3.642
\]

Simpson’s Rule (n = 2):
\[
\text{Area, } A = 0.5/3 \times \left\{ (e^1 - 1) + (e^2 - 1) + 4 \times (e^{1.5} - 1) \right\} = 3.672
\]
\[
\bar{x} A = 0.5/3 \times \left\{ 1 \times (e^1 - 1) + 2 \times (e^2 - 1) + 4 \times 1.5 \times (e^{1.5} - 1) \right\} = 5.898 \Rightarrow \bar{x} = 1.606
\]
\[
\bar{y} A = 0.5/3 \times \left\{ (e^2 - 1) + (e^1 - 1) + 4 \times (e^3 - 1)/2 \right\} = 11.361 \Rightarrow \bar{y} = 3.094
\]
\[
I_y = 0.5/3 \times \left\{ 1^2 \times (e^1 - 1) + 2^2 \times (e^2 - 1) + 4 \times 1.5^2 \times (e^{1.5} - 1) \right\} = 9.768 \Rightarrow r_y = \sqrt{(I_y/A)} = 1.631
\]
\[
I_x = 0.5/3 \times \left\{ (e^3 - 1) + (e^6 - 1) + 4 \times (e^{4.5} - 1)/3 \right\} = 43.199 \Rightarrow r_x = \sqrt{(I_x/A)} = 3.430
\]
Gauss Integration

It integrates a function between limits −1 to +1 using the following formula

\[
\int_{-1}^{1} f(\xi) \, d\xi = \sum A_i f(\xi_i) \tag{1}
\]

where \( \int \) is the integration between −1 to +1 and \( \sum \) is the summation over \( i \).

Here \( \xi_i \)'s are the ordinates (between −1 and +1) where the function is evaluated and \( A_i \)'s are the corresponding coefficients. For integration with different ordinates (for varying accuracy of results), the values of \( \xi_i \) and \( A_i \) from the following table are used.

<table>
<thead>
<tr>
<th>( n )</th>
<th>( \pm \xi_i )</th>
<th>( A_i )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.0</td>
<td>2.0</td>
</tr>
<tr>
<td>2</td>
<td>\pm 0.57735</td>
<td>1.0</td>
</tr>
<tr>
<td>3</td>
<td>\pm 0.77460</td>
<td>0.55556</td>
</tr>
<tr>
<td></td>
<td>0.0</td>
<td>0.88889</td>
</tr>
<tr>
<td>4</td>
<td>\pm 0.86114</td>
<td>0.34785</td>
</tr>
<tr>
<td></td>
<td>\pm 0.33998</td>
<td>0.65215</td>
</tr>
<tr>
<td>5</td>
<td>\pm 0.90618</td>
<td>0.23693</td>
</tr>
<tr>
<td></td>
<td>\pm 0.53847</td>
<td>0.47863</td>
</tr>
<tr>
<td></td>
<td>0.0</td>
<td>0.56889</td>
</tr>
</tbody>
</table>

After getting \( \xi_i \) and \( A_i \), functions can be integrated between \( a \) and \( b \) by coordinate transformation.

\[
\int_{a}^{b} f(x) \, dx = 0.5(b-a) \sum A_i f(x_i) \tag{2}
\]

where \( x_i = 0.5(b+a) + 0.5(b-a) \xi_i \)

The Gaussian integration with \( n \) ordinates is exact for polynomials of degree \((2n-1)\).

Example

Integrate the function \( \cos(x) \) between 0 and \( \pi/2 \).

Solution

Using \( n = 1 \), \( \int f(x) \, dx = 0.5(\pi/2) \left[ A_1 f(x_1) \right] = 0.5(\pi/2) \left[ 2.0 \cos\{0.5(\pi/2)+0.5(\pi/2)\times0\} \right] = 1.11072 \)

Using \( n = 2 \), \( \int f(x) \, dx = 0.5(\pi/2) \left[ A_1 f(x_1) + A_2 f(x_2) \right] \)

\( = 0.5(\pi/2)\left[1.0 \cos\{0.5(\pi/2)-0.5(\pi/2)\times0.57735\}+1.0 \cos\{0.5(\pi/2)+0.5(\pi/2)\times0.57735\} \right] = 0.99847 \)

Using \( n = 3 \), \( \int f(x) \, dx = 1.0000072 \)

[The exact solution is 1.0]
Practice Problems on Numerical Differentiation and Integration

1. The horizontal ground displacement \( S \) recorded at different time \( t \) during an earthquake is shown in the table below. Calculate the ground velocity \( dS/dt \) when \( t = 8.45 \) seconds using (i) Forward Difference Formula, (ii) Backward Difference Formula, (iii) Central Difference Formula. Using the Central Difference Formula, calculate the ground acceleration \( d^2S/dt^2 \) when \( t = 8.50 \) seconds.

<table>
<thead>
<tr>
<th>( t ) (sec)</th>
<th>8.40</th>
<th>8.45</th>
<th>8.50</th>
<th>8.55</th>
</tr>
</thead>
<tbody>
<tr>
<td>( S ) (ft)</td>
<td>0.1757</td>
<td>0.1863</td>
<td>0.1994</td>
<td>0.2141</td>
</tr>
</tbody>
</table>

2. The Bending Moment diagram of a beam is shown below. Draw the shear force and load diagrams using Forward Difference Formula for A, Backward Difference Formula for G and Central Difference Formula for the other points.

3. Carry out integrations between \( x = 1 \) and \( x = 2 \) for the following functions \( f(x) \) using Trapezoidal Rule, Simpson’s Rule and Gauss Integration (with \( n = 2 \)). Compare with exact results whenever possible.
   (i) \( x + \sqrt{x^2 + 1} \), (ii) \( x^3 e^x \), (iii) \( x \log(x) \), (iv) \( e^x \sin(x) \), (v) \( \tan^{-1} x \).
   Calculate \( f'(1.5) \) and \( f''(1.5) \) for each using Central Difference Formula and compare with exact results.

4. Use Trapezoidal Rule to calculate the area shown in the figure below (enclosed by the peripheral points \( A \)-\( E \), \( A' \)-\( E' \) shown with their x and y coordinates) as well as its centroidal coordinates.

5. For the beam loaded as shown in the figure below, calculate the vertical reaction \( R_B \) at support B using Simpson’s Rule [The summation of moments at A due to \( R_B \) and the distributed loads equal to zero].
Numerical Solution of Differential Equations

The Finite Difference Method

This method is based on writing the differentiations in discretized forms; e.g., at point B (Fig. 1)

\[ y' = \frac{dy}{dx} = \frac{(y_2 - y_0)}{2h} \quad \ldots \ldots \text{(i)} \]

\[ y'' = \frac{d^2y}{dx^2} = \frac{(y_2 - 2y_1 + y_0)}{h^2} \quad \ldots \ldots \text{(ii)} \]

Higher order differentiations can be defined similarly.

Equations (i) and (ii) above are called ‘Central Difference Formulae’ because they involve the points on the left and right of the point of interest. Differentiations can also be defined in terms of points on the right or on the left of the point of interest, the formulae being called the ‘Forward Difference Formula’ and the ‘Backward Difference Formulae’ respectively.

For example, the ‘Forward Difference Formula’ for \( y' = \frac{dy}{dx} \) at B is \( y'_B = \frac{(y_2 - y_1)}{h} \quad \ldots \ldots \text{(iii)} \)

while the ‘Backward Difference Formula’ is \( y''_B = \frac{(y_1 - y_0)}{h} \quad \ldots \ldots \text{(iv)} \)

After writing the differential equation by Finite Differences, solution is obtained by applying boundary/initial conditions. The number of conditions is equal to the order of the differential equation.

Example 1

Solve the differential equation \( \frac{dy}{dx} + (\sin x) \ y = 0 \), with \( y(0) = 1 \) (\( x = 0 \) to \( 1 \))

Solution

(a) The exact solution is \( y(x) = e^{-\cos x} \)

(b) Taking two segments between \( x = 0 \) and \( x = 1 \), \( h = (1-0)/2 = 0.5 \)

Let, the values of \( y \) be \( y(0) = y_0 \), \( y(0.5) = y_1 \), \( y(1) = y_2 \Rightarrow y_0 = 1 \)

(1) Using the Forward Difference Formula

At \( x = 0 \) \( \Rightarrow \frac{(y_1 - y_0)}{0.5} + (\sin 0) y_0 = 0 \Rightarrow y_1 = 1 \quad \text{(Exact = 0.8848)} \)

At \( x = 0.5 \) \( \Rightarrow \frac{(y_2 - y_1)}{0.5} + (\sin 0.5) y_1 = 0 \Rightarrow y_2 = 0.7603 \quad \text{(Exact = 0.6315)} \)

(2) Using the Backward Difference Formula

At \( x = 0.5 \) \( \Rightarrow \frac{(y_1 - y_0)}{0.5} + (\sin 0.5) y_1 = 0 \Rightarrow y_1 = 0.8066 \)

At \( x = 1.0 \) \( \Rightarrow \frac{(y_2 - y_1)}{0.5} + (\sin 1.0) y_2 = 0 \Rightarrow y_2 = 0.5678 \)

(3) Using the Central Difference and Backward Difference Formulae

At \( x = 0.5 \), Central Difference \( \Rightarrow \frac{(y_2 - y_0)}{1.0} + (\sin 0.5) y_1 = 0 \)

At \( x = 1.0 \), Backward Difference \( \Rightarrow \frac{(y_2 - y_1)}{1.0} + (\sin 1.0) y_2 = 0 \)

Solving these equations with \( y_0 = 1 \Rightarrow y_1 = 0.8451, y_2 = 0.5948 \)
Example 2

Solve the differential equation \( \frac{dy}{dx} + y = x \), with \( y'(0) = 0 \) (between \( x = 0 \) and \( x = 2 \))

Solution

(a) The exact solution is \( y(x) = x - 1 + e^{-x} \)

(b) Taking four segments between \( x = 0 \) and \( x = 2 \), we have \( h = (2-0)/4 = 0.5 \)

Let, \( y(0) = y_0 \), \( y(0.5) = y_1 \), \( y(1) = y_2 \), \( y(1.5) = y_3 \), \( y(2) = y_4 \)

(1) Using the Forward Difference Formula

Using the Forward Difference Formula at \( x = 0 \) \( \Rightarrow (y_1-y_0)/0.5 = 0 \Rightarrow y_1 = y_0 \)

At \( x = 0 \) \( \Rightarrow (y_1-y_0)/(0.5) + y_0 = 0 \Rightarrow y_0 = 0 \) (Exact \( y_0 = 0 \), \( y_1 = 0.1065 \))

Similarly \( y_2 = 0.25 \), \( y_3 = 0.625 \), \( y_4 = 1.0625 \) (Exact = 0.3679, 0.7231, 1.1353)

(2) Using the Forward & Central Difference Formulae

Using the Forward Difference Formula at \( x = 0 \) \( \Rightarrow (y_1-y_0)/0.5 = 0 \Rightarrow y_1 = y_0 \)

At \( x = 0 \) \( \Rightarrow (y_1-y_0)/(0.5) + y_0 = 0 \Rightarrow y_0 = 0 \)

At \( x = 0.5 \) \( \Rightarrow (y_2-y_0)/(1.0) + y_1 = 0.5 \Rightarrow y_2 = 0.5 \) (Exact = 0.3679, 0.7231, 1.1353)

Example 3

Calculate shear force and bending moment at point (0) of the beam shown below, using \( \frac{d^2M}{dx^2} = -w(x) \), \( M_4 = 0 \), \( M'_4 = 0 \).

![Beam Diagram]

Solution

Let, the bending moments at 3' intervals be \( M_0 \text{ to } M_4 \).

\( \therefore M_4 = 0 \). Assuming imaginary point (5), CDF for \( M'_4 = 0 \Rightarrow M_5 = M_3 \)

\( \therefore \frac{d^2M}{dx^2} = -w(x) \) at (1) \( \Rightarrow (M_0-2M_1+M_2)/3^2 = -1 \), at (2) \( \Rightarrow (M_1-2M_2+M_3)/3^2 = -1.5 \),

at (3) \( \Rightarrow (M_2-2M_3+M_4)/3^2 = -1.5 \), at (4) \( \Rightarrow (M_3-2M_4+M_5)/3^2 = -0.5 \)

\( \therefore M_4 = 0, \text{ and } M_5 = M_3 \Rightarrow M_5 = M_3 = -2.25 \text{ k'} \), \( M_2 = -18.0 \text{ k'} \), \( M_1 = -47.25 \text{ k'} \), \( M_0 = -85.5 \text{ k'} \).

Assuming imaginary point (-1), \( M''_0=-2 \Rightarrow (M_1-2M_0+M_1)/3^2 = -2 \Rightarrow M_1 = -141.75 \text{ k'} \)

\( \therefore \text{Using CDF, } V_0 = (M_1-M_4)/6 = -15.75 \text{ k} \)
Practice Problems on the Solution of Differential Equation by Finite Difference Method

1. Solve the following differential equations between \( x = 0 \) to \( 2 \) for the given boundary conditions. Also compare with exact solutions whenever possible.
   
   (i) \( y' + 2y = \cos(x) \), with \( y(0) = 0 \) [Exact \( y(x) = (2 \cos(x) + \sin(x) - 2e^{-2x})/5 \)]
   
   (ii) \( y' + 2y = \cos(x) \), with \( y'(0) = 0 \) [Exact \( y(x) = (2 \cos(x) + \sin(x) + e^{-2x}/2)/5 \)]
   
   (iii) \( y'' + 4y = \cos(x) \), with \( y(0) = 0, y'(0) = 0 \) [Exact \( y(x) = (\cos(x) - \cos(2x))/3 \)]

2. The acceleration of a body falling through air is given by \( a = dv/dt = 32 - v \). If \( v(0) = 0 \), calculate the velocity \( v \) for \( t = 0.2 \) to \( 1.0 \) @0.2 sec.

3. The acceleration of a body falling through a spring is given by \( a = d^2S/dt^2 = 32 - 2000S \). If \( S(0) = 0, S'(0) = 10 \), calculate the displacement \( S \) for \( t = 0.02 \) to \( 0.10 \) @0.02 sec.

4. The governing differential equation for the axial deformation of an axially loaded pile is given by
   \[
   (600000) w'' - 100 w = 2.5
   \]
   with boundary conditions \( w(0) = 0, w'(15) = 0 \).

   Using 1, 2 and 3 segments, calculate \( w(15) \); i.e., the elongation at the tip of the pile using the Central Difference Formula. Compare the results with the exact solution.

5. Calculate shear force and bending moment at points (1 to 4) for the cantilever beam shown below, using \( d^2M/dx^2 = w(x) \), \( M_0 = 0, M'_0 = 0 \). Compare the results with the exact ones.

6. Calculate shear force at point (0) and bending moment at point (2) for the simply supported beam loaded as shown below, using \( d^2M/dx^2 = w(x) \), \( M_0 = 0, M_4 = 0 \).

7. Given the PDE \( \partial^2y/\partial x^2 + \partial^2y/\partial z^2 = 1 \) and boundary conditions \( y = 0 \) at \( x = \pm 1 \) and \( z = \pm 2 \), calculate \( y \) when \( x = 0 \) and \( z = 0 \).
Numerical Solution of Differential Equations

The Galerkin Method

In this method, a solution satisfying the given boundary conditions is assumed first. The parameters of the assumed solution are determined by minimizing the residual using the least square method.

Example 1

Solve the differential equation \( y' + 2y = \cos(x) \), with \( y(0) = 0 \)

Solution

The differential equation with the given boundary condition has an exact solution

\[
y(x) = \frac{2 \cos(x) + \sin(x) - 2e^{-2x}}{5}
\]

(i) The first assumed solution \( y(x) = ax \Rightarrow R(x) = (1+2x)a - \cos(x) \)

For solution between \( x = 0 \) to \( 1 \), the least-square method of minimizing \( R^2 \) over the domain

\[
\Rightarrow \left\{ (1+2x)^2 \right\} a - \left\{ (1+2x) \cos(x) \right\} = 0 \quad \text{[\( f \) is integration between \( x = 0 \) to \( 1 \)]}
\Rightarrow a = 0.370389 \Rightarrow y(x) = 0.370389 x
\]

(ii) The second solution \( y(x) = bx^2 \Rightarrow R(x) = 2(x+x^2)b - \cos(x) \)

\(.\) Minimizing \( R^2 \) over the domain \( \Rightarrow \left\{ 4(x+x^2)^2 \right\} b - \left\{ 2(x+x^2) \cos(x) \right\} = 0 \)

\Rightarrow b = 0.300439 \Rightarrow y(x) = 0.300439 x^2

(iii) The third solution \( y(x) = ax + bx^2 \Rightarrow R(x) = (1+2x)a + 2(x+x^2)b - \cos(x) \)

\(.\) Minimizing \( R^2 \) over the domain with respect to both \( a \) and \( b \) \( \Rightarrow \)

\[
\left\{ (1+2x)^2 \right\} a + \left\{ 2(1+2x)(x+x^2) \right\} b - \left\{ (1+2x) \cos(x) \right\} = 0
\]

\[
\left\{ (x+x^2)(1+2x) \right\} a + \left\{ 4(x+x^2)^2 \right\} b - \left\{ 2(x+x^2) \cos(x) \right\} = 0
\]

\Rightarrow a = 0.872172, b = -0.543598 \Rightarrow y(x) = 0.872172 x - 0.543598 x^2

Fig. 1: Numerical Solutions for \( y' + 2y = \cos(x) \)
Practice Problems on the Solution of Differential Equation by Galerkin Method

1. Solve the following differential equations between $x = 0$ to $2$ for the given boundary conditions. Also compare with exact solutions.
   (i) $y' + (\sin x) y = 0$, with $y(0) = 1$ [Assume $y(x) = 1 + a_1 x$, Exact $y(x) = e^{-\cos x}$]
   (ii) $y' + y = x$, with $y'(0) = 0$ [Assume $y(x) = a_2 x^2$, Exact $y(x) = x - 1 + e^{-x}$]
   (iii) $y'' + 2y = \cos (x)$, with $y'(0) = 0$ [Assume $y(x) = a_3 + a_2 x^2$, Exact $y(x) = (2 \cos(x)+\sin(x)+e^{-2x}/2)/5$]
   (iv) $y'' + 4y = \cos (x)$, with $y(0) = 0$, $y'(0) = 0$ [Assume $y(x) = a_3 x^2$, Exact $y(x) = (\cos(x)-\cos(2x))/3$]

2. The acceleration of a body falling through air is given by $a = \frac{dv}{dt} = 32 - v$. If $v(0) = 0$, calculate the velocity $v$ for $t = 0.2$ to $1.0$ [Assume $v(t) = a_1 t$, Exact $v(t) = 32(1-e^{-t})$].

3. The acceleration of a body falling through a spring is given by $a = \frac{d^2S}{dt^2} = 32-2000 S$. If $S(0) = 0$, $S'(0) = 10$, calculate the displacement $S$ for $t = 0.02$ to $0.10$ [Assume $S(t) = 10t + a_2 t^2$, Exact $S(t) = 0.016\{1-\cos(44.72 t)} + 0.2236 \sin(44.72 t)$].

4. The governing differential equation for the axial deformation of an axially loaded pile is given by
   \[(60000) w'' - 100 w = 2.5\]
   with boundary conditions $w(0) = 0$, $w'(15) = 0$. Calculate $w(15)$; i.e., the elongation at the tip of the pile assuming (i) $w(x) = a_1 \sin(\pi x/30)$, (ii) $w(x) = a_1 (x - x^2/30)$. Compare the results with the exact solution $w(15) = -0.004052$.

5. Draw the shear force and bending moment diagrams for the cantilever beam shown below, using $\frac{d^2M}{dx^2} = w(x)$, $M(0) = 0$, $M'(0) = 0$. Assume $M(x) = a_3 x^2$ and compare the results with the exact ones.

   ![Cantilever Beam Diagram](image)

6. Draw the shear force and bending moment diagrams for the simply supported beam loaded as shown below, using $\frac{d^2M}{dx^2} = w(x)$, $M(0) = 0$, $M(12) = 0$ [Assume $M(x) = a_3 \sin(\pi x/12)$].

   ![Simply Supported Beam Diagram](image)

7. Given the PDE $\frac{\partial^2 y}{\partial x^2} + \frac{\partial^2 y}{\partial z^2} = 1$ and boundary conditions $y = 0$ at $x = \pm 1$ and $z = \pm 2$, calculate $y$ when $x = 0$ and $z = 0$ [Assume $y(x) = a \cos(\pi x/2)\cos(\pi z/4)$].