MM597

ADVANCED NUMERICAL METHODS IN ENGINEERS

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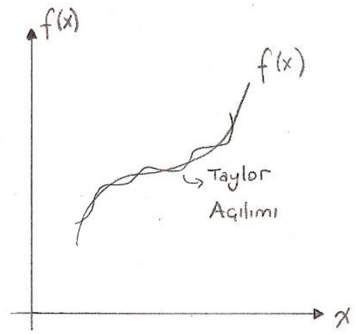
1. APPROXIMATE SOLUTIONS OF EQUATIONS

Sometimes, we encounter problems such as finding the roots of equations of the form $f(x)=0$

1.1. Newton-Rapson Method

To find the roots of an equation given by the function $f(x)=0$, let's open the Taylor series at $x = x_0$. So we can write it as $a_n x^n + a_{n-1} x^{n-1} + \ldots + a_0$



For the Fourier series expansion, it can be written as:

$$f(x) = a_n \cos(b_n x) + c_n \sin(d_n x) + a_{n-1} \cos(b_{n-1} x) + c_{n-1} \sin(d_{n-1} x) + \ldots$$

If we write Taylor Series expansion; $f(x) = f(x_0) + (x - x_0) f'(x_0) + \dfrac{(x-x_0)^2}{2!} f''(x_0) + \ldots$

In this series, at $x=0$ the McLauren series occurs. If we solve this equation, x_0 is the closest value to root. Therefore, the 3rd term and after converge to 0.

$$\Rightarrow \quad f(x) = f(x_0) + (x - x_0) f'(x_0)$$

$$\downarrow \qquad\qquad f(x)=0$$

$$0 = f(x_0) + (x - x_0) f'(x_0)$$

=> $x = x_0 - \frac{f(x_0)}{f'(x_0)}$ => $\boxed{x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}}$ (Newton-Raphson Method)

Example-1: Find the roots of the equation given by $x^2 - 2 = 0$

$$x_{1,2} = \mp\sqrt{2} = \mp 1.414213562$$

$$f(x) = x^2 - 2$$

$$f'(x) = 2x$$

=> $x_{n+1} = x_n - \frac{x_n^2 - 2}{2x_n}$ (we can take any value as an first approximation)

If we choose $x_0 = 1$, as the first approximation value.

=> $x_1 = 1 - \frac{1^2 - 2}{2*1} = 1.5$

$$x_2 = 1.5 - \frac{1.5^2 - 2}{2*1.5} = 1.4166667$$

$$x_3 = 1.4166667 - \frac{1.4166667^2 - 2}{2*1.4166667} = 1.4142157$$

$$x_4 = 1.4142157 - \frac{1.4142157^2 - 2}{2*1.4142157} = 1.4142143$$

$x_5 = 1.4142143 - \frac{1.4142143^2 - 2}{2*1.4142143} = 1.4142136$ * Solution

$$x_6 = 1.4142136$$

Note: The found root converges to the root closest to the initially accepted value.

Example-2: Find the roots of the equation given by $e^{x^2} - x^3 + 3.x - 4 = 0$

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

$$f'(x) = 2xe^{x^2} - 3x^2 + 3$$

$x_0 = 0.5$ is chosen as a first approximation,

$$x_1 = x_0 - \frac{f(x_0)}{f'(x_0)} = 0.5 - \frac{e^{(0.5)^2} - (0.5)^3 + 3*(0.5) - 4}{2*0.5*e^{(0.5)^2} - 3*(0.5)^2 + 3}$$

=> $x_1 = 0.5 - \frac{e^{(0.5)^2} - (0.5)^3 + 3*(0.5) - 4}{2*0.5*e^{(0.5)^2} - 3*(0.5)^2 + 3} = 0.8794467$ bulunarak iterasyona devam edilir.

$$x_2 = 0.8794467 - \frac{e^{(0.8794467)^2} - (0.8794467)^3 + 3*(0.8794467) - 4}{2*0.8794467*e^{(0.8794467)^2} - 3*(0.8794467)^2 + 3} = 0.8515428$$

$x_3 = 0.8515428 - \frac{e^{(0.8515428)^2} - (0.8515428)^3 + 3*(0.8515428) - 4}{2*0.8515428*e^{(0.8515428)^2} - 3*(0.8515428)^2 + 3} = 0.851049$ *Çözüm

$$x_4 = 0.851049$$

The root found is the closest root to 0.5.

1.2. Newton's Modified Method

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

$$\boxed{u'(x_n) = 1 - \frac{f(x_n) * f''(x_n)}{[f'(x_n)]^2}}$$

In this method, the solution can be reached more easily by reducing the number of iterations. However, it is not preferred because the quadratic derivative of the function is used during the solution.

1.3. Secant Method

If we define the derivative; $f'(x) = \lim_{x_n - x_{n-1} \to 0} \frac{f(x_n) - f(x_{n-1})}{x_n - x_{n-1}}$

When we apply this definition to the Newton-Rapson model, we obtain the Secant method equation:

=> $$\boxed{x_{n+1} = x_n - \frac{f(x_n)}{\left[f(x_n) - f(x_{n-1})\right]/(x_n - x_{n-1})}}$$

$$x_{n+1} = x_n - \frac{f(x_n) * (x_n - x_{n-1})}{\left[f(x_n) - f(x_{n-1})\right]}$$

In this method, we do not take the derivative of the function, but instead of one initial value, two initial values must be chosen.

Homework:

1) Find $\sqrt[5]{83}$ $\left(f(x) = x^5 - 83\right)$; by using all methods with precision up to the 6th digit.

2) Find the root of the equation $f(x) = x^2 - 2e^{-x} * x^3 - e^{-3x}$ by taking initial values as $x_0 = 1$ and $x_{-1} = 2$ (by using all methods).

3) Find the root of the equation $\sin(x^3 + 2) = \frac{1}{x}$ by taking initial values as $x_0 = 1$ and $x_{-1} = 3$ (by using all methods).

2. SOLUTION OF LINEAR EQUATIONS AND INVERSION OF THE MATRIX

$$C = \begin{bmatrix} c_{11} & c_{12} & c_{13} & c_{14} \\ c_{21} & c_{22} & c_{23} & c_{24} \\ c_{31} & c_{32} & c_{33} & c_{34} \\ c_{41} & c_{42} & c_{43} & c_{44} \end{bmatrix}$$

4*4 matrix

$c_{11}, c_{22}, c_{33}, c_{44}$ diagonal terms

If $C_{ij} = C_{ji}$, then this matrix is a symmetric matrix

$$C = \begin{bmatrix} c_{11} & c_{12} & c_{13} & c_{14} \\ 0 & c_{22} & c_{23} & c_{24} \\ 0 & 0 & c_{33} & c_{34} \\ 0 & 0 & 0 & c_{44} \end{bmatrix}$$

This matrix is called the upper trigonal matrix.

In the opposite case, it is called the lower trigonal matrix.

$$C = \begin{bmatrix} c_{11} & 0 & 0 & 0 \\ 0 & c_{22} & 0 & 0 \\ 0 & 0 & c_{33} & 0 \\ 0 & 0 & 0 & c_{44} \end{bmatrix}$$

Diagonal matrix

$$I = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

Unit matrix

$$C = \begin{bmatrix} c_{11} & c_{12} & 0 & 0 \\ c_{21} & c_{22} & c_{23} & 0 \\ 0 & c_{32} & c_{33} & c_{34} \\ 0 & 0 & c_{43} & c_{44} \end{bmatrix}$$

Band type matrix [Tri-diagonal matrix]

Some Matrix Properties

1) The sum of two matrices (such as A and B) is defined as long as their dimensions are the same.

$$S = A + B = B + A$$

$$s_{ij} = a_{ij} + b_{ij} = b_{ij} + a_{ij}$$

$$\begin{bmatrix} 1 & 2 \\ 0 & 1 \\ 3 & 0 \end{bmatrix} + \begin{bmatrix} 2 & 1 \\ 4 & 0 \\ 1 & 3 \end{bmatrix} = \begin{bmatrix} 3 & 3 \\ 4 & 1 \\ 4 & 3 \end{bmatrix}$$

2) The difference of two matrices of the same size,

$$S = A - B = -B + A$$

$$\begin{bmatrix} 1 & 2 \\ 0 & 1 \\ 3 & 0 \end{bmatrix} - \begin{bmatrix} 2 & 1 \\ 4 & 0 \\ 1 & 3 \end{bmatrix} = \begin{bmatrix} -1 & 1 \\ -4 & 1 \\ 2 & -3 \end{bmatrix}$$

3) In multiplication of two matrices, if the number of columns in the first matrix is equal to the number of rows in the second matrix, the multiplication operation is defined.

$$S = A * B \neq B * A$$

$$\begin{bmatrix} 1 & 2 \\ 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 2 & 1 \\ 1 & 0 \end{bmatrix} = \begin{bmatrix} 1*2+2*1 & 1*1+2*0 \\ 0*2+1*1 & 0*1+1*0 \\ 1*2+0*1 & 1*1+0*0 \end{bmatrix} = \begin{bmatrix} 4 & 1 \\ 1 & 0 \\ 2 & 1 \end{bmatrix}$$

General formula; $P_{ij} = \sum_{k=1}^{n} a_{ik} b_{kj}$

4) When a matrix is multiplied by the unit matrix, the result is the matrix itself.

$$AI = A = IA$$

5) If the inverse of the C matrix C^{-1} exists, $C.C^{-1} = I$ and $\left(C^{-1}\right)^{-1} = C$ (For the inverse to happen, the matrix must be a square matrix and its determinant must be different from "0")

$$C_{ij}^{-1} = \frac{cofactor\, of\ C_{ij}}{|C|} = \frac{(-1)^{i+j} M_{ji}}{|C|}$$

Example-3: Find the inverse of $C = \begin{bmatrix} 8 & 0 & 1 \\ 3 & -2 & 1 \\ 1 & 4 & 0 \end{bmatrix}$

If we calculate the determinant,

$$|C| = \begin{bmatrix} 8 & 0 & 1 \\ 3 & -2 & 1 \\ 1 & 4 & 0 \end{bmatrix}\begin{matrix} 8 & 0 \\ 3 & -2 \\ 1 & 4 \end{matrix} = \left[(8*-2*0)+(0*1*1)+(1*3*4)\right]-\left[(1*-2*1)+(8*1*4)+(0*3*0)\right]$$

$$|C| = \begin{bmatrix} 8 & 0 & 1 \\ 3 & -2 & 1 \\ 1 & 4 & 0 \end{bmatrix}\begin{matrix} 8 & 0 \\ 3 & -2 \\ 1 & 4 \end{matrix} = 12-30 = -18$$

$$c_{11}^{-1} = \frac{(-1)^{1+1} M_{11}}{|C|} = \frac{1*\begin{vmatrix} -2 & 1 \\ 4 & 0 \end{vmatrix}}{-18} = \frac{-4}{-18} = \frac{4}{18}$$

$$c_{12}^{-1} = \frac{(-1)^{1+2} M_{21}}{|C|} = \frac{-1*\begin{vmatrix} 0 & 1 \\ 4 & 0 \end{vmatrix}}{-18} = \frac{4}{-18} = -\frac{4}{18}$$

$$c_{13}^{-1}=\frac{(-1)^{1+3}M_{31}}{|C|}=\frac{1*\begin{vmatrix}0 & 1\\ -2 & 1\end{vmatrix}}{-18}=\frac{2}{-18}=-\frac{2}{18}$$

$$c_{21}^{-1}=\frac{(-1)^{1+2}M_{12}}{|C|}=\frac{-1*\begin{vmatrix}3 & 1\\ 1 & 0\end{vmatrix}}{-18}=\frac{1}{-18}=-\frac{1}{18}$$

$$c_{22}^{-1}=\frac{(-1)^{2+2}M_{22}}{|C|}=\frac{1*\begin{vmatrix}8 & 1\\ 1 & 0\end{vmatrix}}{-18}=\frac{-1}{-18}=\frac{1}{18}$$

$$c_{23}^{-1}=\frac{(-1)^{2+3}M_{32}}{|C|}=\frac{-1*\begin{vmatrix}8 & 1\\ 3 & 1\end{vmatrix}}{-18}=\frac{-5}{-18}=\frac{5}{18}$$

$$c_{31}^{-1}=\frac{(-1)^{3+1}M_{13}}{|C|}=\frac{1*\begin{vmatrix}3 & -2\\ 1 & 4\end{vmatrix}}{-18}=\frac{14}{-18}=-\frac{14}{18}$$

$$c_{32}^{-1}=\frac{(-1)^{3+2}M_{23}}{|C|}=\frac{-1*\begin{vmatrix}8 & 0\\ 1 & 4\end{vmatrix}}{-18}=\frac{-32}{-18}=\frac{32}{18}$$

$$c_{33}^{-1}=\frac{(-1)^{3+3}M_{33}}{|C|}=\frac{1*\begin{vmatrix}8 & 0\\ 3 & -2\end{vmatrix}}{-18}=\frac{-16}{-18}=\frac{16}{18}$$

$$C^{-1}=\frac{1}{18}\begin{bmatrix}4 & -4 & -2\\ -1 & 1 & 5\\ -14 & 32 & 16\end{bmatrix}$$

6) The determinant of a matrix of n*n dimensions is $|C| = \sum_{j=1}^{n} (-1)^{k+j} c_{kj} M_{kj}$. In this formula, a solution can be made by considering the desired row or column in the matrix. Selecting the row or column with the highest number of "0" is convenient for analysis.

Example-4: Calculate the determinant of $C = \begin{bmatrix} -3 & 1 & 16 & -8 \\ 0 & 1 & 14 & 0 \\ 0 & 3 & 0 & 1 \\ 0 & 14 & 6 & 0 \end{bmatrix}$

The analysis will be made by considering the 1st column with the maximum number of "0".

$$C = \begin{bmatrix} -3 & 1 & 16 & -8 \\ 0 & 1 & 14 & 0 \\ 0 & 3 & 0 & 1 \\ 0 & 14 & 6 & 0 \end{bmatrix} = (-1)^{1+1}(-3)\begin{vmatrix} 1 & 14 & 0 \\ 3 & 0 & 1 \\ 14 & 6 & 0 \end{vmatrix} + (-1)^{1+2}(0)\begin{vmatrix} 1 & 16 & -8 \\ 3 & 0 & 1 \\ 14 & 6 & 0 \end{vmatrix} + (-1)^{1+3}(0)\ldots$$

=> $$= -3\begin{vmatrix} 1 & 14 & 0 \\ 3 & 0 & 1 \\ 14 & 6 & 0 \end{vmatrix} = -3\left[(-1)^{2+3}(1)\begin{vmatrix} 1 & 14 \\ 14 & 6 \end{vmatrix}\right] = -3[-1*(1*6-14*14)] = 3*(6-196) = -570$$

<u>Matrix Representation of Systems of Linear Equations</u>

$$c_{11}x_1 + c_{12}x_2 + c_{13}x_3 + c_{14}x_4 = r_1$$

$$c_{21}x_1 + c_{22}x_2 + c_{23}x_3 + c_{24}x_4 = r_2$$

$$c_{31}x_1 + c_{32}x_2 + c_{33}x_3 + c_{34}x_4 = r_3$$

$$c_{41}x_1 + c_{42}x_2 + c_{43}x_3 + c_{44}x_4 = r_4$$

=> $$\begin{bmatrix} c_{11} & c_{12} & c_{13} & c_{14} \\ c_{21} & c_{22} & c_{23} & c_{24} \\ c_{31} & c_{32} & c_{33} & c_{34} \\ c_{41} & c_{42} & c_{43} & c_{44} \end{bmatrix}\begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} r_1 \\ r_2 \\ r_3 \\ r_4 \end{bmatrix}$$

$$C.X = R$$

Note: The determinant of a matrix whose two rows or two columns are the same is always 0.

The classical solution of this system of equations is done by Cramer's rule.

$$X_k = \frac{\det(C_k)}{\det(C)}$$

C_k ; is the resulting matrix with the k[th] column replaced with R. The reason for not using this method is the total number of operations consisting of addition, subtraction, multiplication and division operations for each calculation. Approximately $O(N^4)$ operation is needed.

$$C.X = R$$

=> $$C^{-1}.C.X = C^{-1}.R$$

$$I.X = C^{-1}.R$$

$$X = C^{-1}.R$$

Example–5: Solve the following system of equations using Cramer's rule.

$$x_1 - 3x_2 - 4x_3 = 1$$

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

$$x_2 - 3x_3 = 5$$

$$\begin{vmatrix} 1 & -3 & -4 \\ -1 & 1 & -3 \\ 0 & 1 & -3 \end{vmatrix} \begin{vmatrix} x_1 \\ x_2 \\ x_3 \end{vmatrix} = \begin{vmatrix} 1 \\ 14 \\ 5 \end{vmatrix}$$

If we calculate its determinant,

$$\left|\begin{array}{ccc|cc} 1 & -3 & -4 & 1 & -3 \\ -1 & 1 & -3 & -1 & 1 \\ 0 & 1 & -3 & 0 & 1 \end{array}\right| = 1+12 = 13$$

$$x_1 = \frac{\left|\begin{array}{ccc|cc} 1 & -3 & -4 & 1 & -3 \\ 14 & 1 & -3 & 14 & 1 \\ 5 & 1 & -3 & 5 & 1 \end{array}\right|}{13} = \frac{-117}{13} = -9$$

$$x_2 = \frac{\left|\begin{array}{ccc|cc} 1 & 1 & -4 & 1 & 1 \\ -1 & 14 & -3 & -1 & 14 \\ 0 & 5 & -3 & 0 & 5 \end{array}\right|}{13} = \frac{-10}{13}$$

$$x_3 = \frac{\left|\begin{array}{ccc|cc} 1 & -3 & 1 & 1 & -3 \\ -1 & 1 & 14 & -1 & 1 \\ 0 & 1 & 5 & 0 & 1 \end{array}\right|}{13} = \frac{-25}{13}$$

GAUSS VE GAUSS-JORDAN ELEMINATION METHODS

$$c_{11}x_1 + c_{12}x_2 + c_{13}x_3 + c_{14}x_4 = r_1$$

$$c_{21}x_1 + c_{22}x_2 + c_{23}x_3 + c_{24}x_4 = r_2$$

$$c_{31}x_1 + c_{32}x_2 + c_{33}x_3 + c_{34}x_4 = r_3$$

$$c_{41}x_1 + c_{42}x_2 + c_{43}x_3 + c_{44}x_4 = r_4$$

$$
=> \quad \begin{bmatrix} c_{11} & c_{12} & c_{13} & c_{14} \\ c_{21} & c_{22} & c_{23} & c_{24} \\ c_{31} & c_{32} & c_{33} & c_{34} \\ c_{41} & c_{42} & c_{43} & c_{44} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} r_1 \\ r_2 \\ r_3 \\ r_4 \end{bmatrix}
$$

$$C.X = R$$

If we divide the first row of the matrix by c_{11},

$$
=> \quad \begin{bmatrix} 1 & c'_{12} & c'_{13} & c'_{14} \\ c_{21} & c_{22} & c_{23} & c_{24} \\ c_{31} & c_{32} & c_{33} & c_{34} \\ c_{41} & c_{42} & c_{43} & c_{44} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} r'_1 \\ r_2 \\ r_3 \\ r_4 \end{bmatrix}
$$

After this step, we will multiply the first row by c_{21} and subtract from the second row, multiply the first row by c_{31} and subtract from the third row and multiply the first row by c_{41} and subtract from the fourth row, the matrix becomes:

$$
=> \quad \begin{bmatrix} 1 & c'_{12} & c'_{13} & c'_{14} \\ 0 & c'_{22} & c'_{23} & c'_{24} \\ 0 & c'_{32} & c'_{33} & c'_{34} \\ 0 & c'_{42} & c'_{43} & c'_{44} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} r'_1 \\ r'_2 \\ r'_3 \\ r'_4 \end{bmatrix}
$$

If we repeat this sequence of operations for the second row (Dividing second row by c'_{22}, multiplying second row by c'_{32} and subtracting from third row; multiplying second row by c'_{42} and subtracting from fourth row) the matrix becomes:

$$=> \begin{bmatrix} 1 & c'_{12} & c'_{13} & c'_{14} \\ 0 & 1 & c''_{23} & c''_{24} \\ 0 & 0 & c''_{33} & c''_{34} \\ 0 & 0 & c''_{43} & c''_{44} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} r_1' \\ r_2'' \\ r_3'' \\ r_4'' \end{bmatrix}$$

When the same operations are done for the 3rd and 4th rows,

$$=> \begin{bmatrix} 1 & c'_{12} & c'_{13} & c'_{14} \\ 0 & 1 & c''_{23} & c''_{24} \\ 0 & 0 & 1 & c'''_{34} \\ 0 & 0 & 0 & c'''_{44} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} r_1' \\ r_2'' \\ r_3''' \\ r_4''' \end{bmatrix}$$

$$=> \begin{bmatrix} 1 & c'_{12} & c'_{13} & c'_{14} \\ 0 & 1 & c''_{23} & c''_{24} \\ 0 & 0 & 1 & c'''_{34} \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} r_1' \\ r_2'' \\ r_3''' \\ r_4'''' \end{bmatrix}$$

$$=> \quad x_4 = r_4''''$$

$$x_3 + c'''_{34}.x_4 = r_3''' \qquad => \qquad x_3 = r_3''' - c'''_{34}.x_4$$

$$x_2 + c''_{23}.x_3 + c''_{24}.x_4 = r_2'' \qquad => \qquad x_2 = r_2'' - c''_{23}.x_3 - c''_{24}.x_4$$

$$x_1 + c'_{12}.x_2 + c'_{13}.x_3 + c'_{14}.x_4 = r_1' \;=>\; x_1 = r_1' - c'_{12}.x_2 - c'_{13}.x_3 - c'_{14}.x_4$$

When the solution is made with the Gauss-Jordon method, the following matrix system is formed,

$$=> \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} r_1'''' \\ r_2'''' \\ r_3'''' \\ r_4'''' \end{bmatrix}$$

In this method, the number of operations is 1.5 times higher than the Gaussian elimination method. For this reason, the Gaussian elimination method is preferred.

Example: $\begin{bmatrix} 3 & 1 & -1 \\ 1 & 4 & 1 \\ 2 & 1 & 2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 2 \\ 12 \\ 10 \end{bmatrix}$ Solve the equation with Gauss and Gauss-Jordan method.

If we start the solution with the Gauss method,

Step 1. Operations related to the first row,

$$\begin{bmatrix} 1 & 1/3 & -1/3 \\ 1 & 4 & 1 \\ 2 & 1 & 2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 2/3 \\ 12 \\ 10 \end{bmatrix}$$

$$=> \quad \begin{bmatrix} 1 & 1/3 & -1/3 \\ 0 & 11/3 & 4/3 \\ 0 & 1/3 & 8/3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 2/3 \\ 34/3 \\ 26/3 \end{bmatrix}$$

Step 2. Operations related to the second row,

$$=> \quad \begin{bmatrix} 1 & 1/3 & -1/3 \\ 0 & 1 & 12/33 \\ 0 & 1/3 & 8/3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 2/3 \\ 34/11 \\ 26/3 \end{bmatrix}$$

$$=> \quad \begin{bmatrix} 1 & 1/3 & -1/3 \\ 0 & 1 & 4/11 \\ 0 & 0 & 84/33 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 2/3 \\ 34/11 \\ 252/33 \end{bmatrix}$$

Step 3. Operations related to the third row,

$$=> \quad \begin{bmatrix} 1 & 1/3 & -1/3 \\ 0 & 1 & 4/11 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 2/3 \\ 34/11 \\ 3 \end{bmatrix}$$

$$x_3 = 3$$

$$x_2 + x_3 \frac{4}{11} = \frac{34}{11} \qquad => \qquad x_2 = 2$$

$$x_1 + x_2 \frac{1}{3} - x_3 \frac{1}{3} = \frac{2}{3} \qquad => \qquad x_1 = 1$$

The final set of equations to be obtained when solving with Gauss-Jordan is below,

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix}$$

Homework:

1) $\begin{bmatrix} b_1 & c_1 & 0 & 0 & 0 & 0 & 0 \\ a_2 & b_2 & c_2 & 0 & . & . & 0 \\ 0 & a_3 & b_3 & c_3 & . & . & 0 \\ 0 & . & . & . & . & . & 0 \\ 0 & . & . & . & . & . & 0 \\ 0 & . & & . & a_{n-1} & b_{n-1} & c_{n-1} \\ 0 & 0 & 0 & 0 & 0 & a_n & b_n \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ . \\ . \\ x_{n-1} \\ x_n \end{bmatrix} = \begin{bmatrix} r_1 \\ r_2 \\ r_3 \\ . \\ . \\ r_{n-1} \\ r_n \end{bmatrix}$ Develop an algorithm for this system

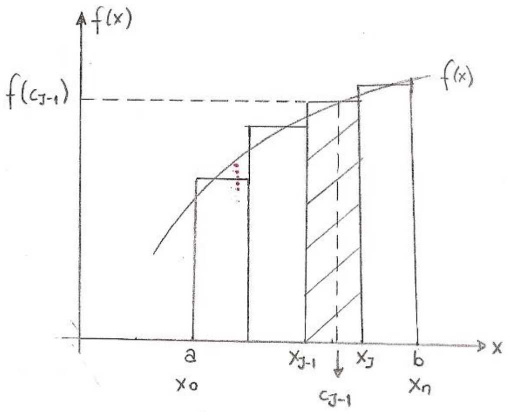
that can be solved using the Gaussian elimination technique.

2) $\begin{bmatrix} 3 & -5 & 47 & 20 \\ 11 & 16 & 17 & 10 \\ 56 & 22 & 11 & -18 \\ 17 & 66 & -12 & 7 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} 18 \\ 26 \\ 34 \\ 82 \end{bmatrix}$ Solve the system of equations.

Results: $x_1 = -1.076888$, $x_2 = 1.99028$, $x_3 = 1.474477$ and $x_4 = -1.906078$

3) NUMERICAL INTEGRATION

3.1) Rectangles Integration Rule



$$\int_a^b f(x)dx = \sum_{j=1}^{n} f(c_{j-1})(x_j - x_{j-1})$$

$h = \dfrac{b-a}{n}$ (pitch range)

$$\int_a^b f(x)dx \cong h[f(c_0) + f(c_1) + \dots\dots + f(c_{n-1})]$$

If $c_{j-1} = x_{j-1}$,

$$\int_a^b f(x)dx \cong h[f(x_0) + f(x_1) + f(x_2) + \dots\dots + f(x_{n-1})]$$

If $c_{j-1} = \dfrac{x_j + x_{j-1}}{2}$, (that is generally used)

$$\int_a^b f(x)dx \cong h[f(c_0) + f(c_1) + \dots\dots + f(c_{n-1})]$$

The order of error that occurs as a result of the integral solved in this method,

m If minimum value of $f''(x)$

M If maximum value of $f''(x)$; the error, ε is in range of

$$\frac{m(b-a)^3}{12n^2} \le \varepsilon \le \frac{M(b-a)^3}{12n^2}$$

If we interpret this formula; It is seen that the error decreases as the number of intervals $1/n^2$, in other words, when h (step interval) increases, the error also increases.

Example: $\int_1^4 x^2 dx = ?$, for n=2, obtain the approximate result of the integral using the rectangular integration method.

$$\int_1^4 x^2 dx = \left.\frac{x^3}{3}\right|_1^4 = 21$$

For $n = 2$,

$x_j = x_0 + j.h \qquad , \; j = 0,1,2,......,n$

$$h = \frac{b-a}{n} = \frac{4-1}{2} = 1.5$$

$x_j = 1 + 1.5j \qquad , \; j = 0,1,2$

$x_0 = 1$

$x_1 = 2.5$

$x_2 = 4$

=> $$\int_1^4 x^2 dx \approx h\left[f(c_0) + f(c_1)\right]$$

$$c_{j-1} = \frac{x_j + x_{j-1}}{2}$$

$$c_0 = \frac{x_1 + x_0}{2} = \frac{1 + 2.5}{2} = 1.75$$

$$c_1 = \frac{x_2 + x_1}{2} = \frac{2.5 + 4}{2} = 3.25$$

$$\int_1^4 x^2 dx \approx h\left[f(c_0) + f(c_1)\right] \cong 1.5\left[(1.75)^2 + (3.25)^2\right] \cong 20.4375$$

As the number of steps, n is increased, the process gets closer to the correct result.

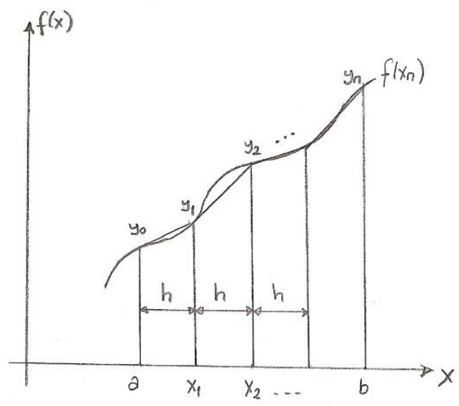
n	$\int_1^4 x^2 dx$
2	20.4375
4	20.859375
10	20.9775
50	20.9991
100	20.999775

Example: $\int_0^{\pi/2} e^{-x^2} \sin(x^2+1)dx = ?$

Solution; for $n = 100$ $\int_0^{\pi/2} e^{-x^2} \sin(x^2+1)dx = 0.7484696904$ and

For $n = 200$ $\int_0^{\pi/2} e^{-x^2} \sin(x^2+1)dx = 0.748468314$

3.2) Trapezoidal Integration Rule



=> $$f(x)=\frac{1}{2}(y_0+y_1)(x_1-x_0)+\frac{1}{2}(y_1+y_2)(x_2-x_1)+......+\frac{1}{2}(y_{n-1}+y_n)(x_n-x_{n-1})$$

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

Formula of trapezoidal integration rule

$$\int_a^b f(x)dx \cong \frac{1}{2}h[y_o+2y_1+2y_2+......+2y_{n-1}+y_n] \quad *$$

Error, $E=\frac{(b-a)}{12}f''(c)h^2 \qquad a\le c\le b$

$$\int_a^b f(x)dx \cong \frac{1}{2}h[y_o+2y_1+2y_2+......+2y_{n-1}+y_n]+O(h^2)$$

Example: For n=2 by using trapezoidal integration rule, find the approximate value of $\int_1^4 x^2dx=?$.

For $n=2$,

$x_j=x_0+j.h \qquad , \; j=0,1,2,......,n$

$h=\frac{b-a}{n}=\frac{4-1}{2}=1.5$

$x_j = 1 + 1.5j \qquad , \; j = 0,1,2$

$x_0 = 1 \qquad\qquad x_1 = 2.5 \qquad\qquad x_2 = 4$

$$\int_1^4 f(x)dx \cong \frac{1}{2}h[y_o + 2y_1 + y_2] \cong \frac{1.5}{2}\left[1^2 + 2.(2.5)^2 + 4^2\right]$$

=> $\int_1^4 f(x)dx \cong 22.125$

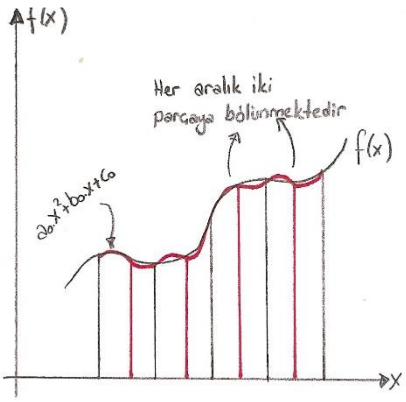
As the number of steps is increased, the process gets closer to the correct result.

n	$\int_1^4 x^2 dx$
2	22.125
4	21.28125
10	21.045
50	21.00180
100	21.00045

Example: $\int_0^{\pi/2} \sin(x^2)dx = ?$

n	Rectangular Rule	Trapezoidal Rule
2	0.89293919	0.69947699
4	0.84420228	0.79620809
10	0.83064857	0.82305960
50	0.82821727	0.82791446
100	0.82814156	0.82806586

3.3) Simpson Integration Rule



In this method, each interval divided between a and b is also divided into two within itself. It is tried to approach the solution by defining a quadratic curve passing thorough each point. Here, as we can see in the error expression, the error rates decrease with respect to order of h^4.

=>

$$\int_a^b f(x)dx \cong \frac{h}{3}\left[y_0+4y_1+2y_2+4y_3+2y_4+......+2y_{n-2}+4y_{n-1}+y_n\right]+O\left(h^4\right)$$

Error, $$E=\frac{(b-a)}{180}f''''(c).h^4=O\left(h^4\right) \qquad a \le c \le b$$

Example: $\int_1^4 x^2dx=?$, for n=2, obtain the integral using Simpson's integration method.

For $n=2$,

$x_j=x_0+j.h \qquad , \quad j=0,1,2,......,n$

$$h=\frac{b-a}{n}=\frac{4-1}{2}=1.5$$

$x_j=1+1.5j \qquad , \quad j=0,1,2$

$x_0=1$

$x_1 = 2.5$

$x_2 = 4$

$$\int_a^b f(x)dx \cong \frac{h}{3}\left[y_0 + 4y_1 + y_2\right]$$

$$\int_a^b f(x)dx \cong \frac{1.5}{3}\left[1^2 + 4(2.5)^2 + 4^2\right]$$

=> $\int_1^4 f(x)dx = 21$

Example: $\int_0^1 \frac{dx}{\sqrt{2\sin^2 x}} = ?$ Find the result of the integration according to all three rules?

Solution:

n	Rectangular Rule	Trapezoidal Rule	Simpson's Rule
2	0.76260967	0.77253221	0.7655945
10	0.76582073	0.76620815	0.76594906
50	0.76594477	0.76596025	0.76594992
100	0.76594864	0.76595251	0.76594993

3.4) Romberg Integration Rule

This rule will not be used in this course.

HOMEWORK

1) $\int_0^{\pi} \sin(x)dx = ?$

2) $\int_0^{\pi} \ln(5 - 4.\cos(x))dx = ?$

3) $\int_0^{0.8} e^{-x^2} dx = ?$

4) $\int_{0.1}^{1} \frac{\ln(x)}{x+1} dx = ?$

By choosing n=100, solve the integrals using all the methods.

3.5) Gauss-Legendre Quadrature and Integration

The aim of the method, to calculate the integral $\int_{-1}^{1} f(x)dx$. In the formula given below, x_k and w_k values are gauss quadratures. x_k's represent the roots of the Legendre polynomial and the w_k's represent the weight functions dependent on these roots. The limits of integral are between -1 and 1.

$$\int_{-1}^{1} f(x)dx \approx w_1.f(x_1)+w_2.f(x_2)+......+w_n f(x_n) \cong \sum_{k=1}^{n} w_k.f(x_k) \qquad *$$

Legendre Polynomials,

$$P_n(x)=\frac{1}{2^n.n!}\frac{d^n}{dx^n}\left\{\left[x^2-1\right]^n\right\}$$ can be calculated by "Rodriguez Formula".

$$P_0(x)=1$$

$$P_1(x)=x$$

$$P_2(x)=\frac{1}{2}\left(3x^2-1\right)$$

$$P_3(x)=\frac{1}{2}\left(5x^3-3x\right)$$

$$P_4(x)=\frac{1}{8}\left(35x^4-30x^2+3\right)$$

.

.

If two previous Legendre polynomials are known, the remaining Legendre polynomials can be calculated by the "recurrence relation".

Recurrence relation : $(n+1).P_{n+1}(x) - (2n+1)x.P_n(x) + n.P_{n-1}(x) = 0$

If this formula is applied for n=1,

$$2.P_2(x) - 3x.P_1(x) + P_0(x) = 0$$

=> $2.P_2(x) = 3x.P_1(x) - P_0(x) = 3x.x - 1$

=> $P_2(x) = \dfrac{3x^2 - 1}{2}$

Weight Function : $w_k = \boxed{\dfrac{2\left(1 - x_k{}^2\right)}{n^2\left[P_{n-1}(x_k)\right]^2}}$

Example: Find the Gauss quadratures for n=3.

$P_3(x) = \dfrac{1}{2}\left(5x^3 - 3x\right) = 0$ => $5x^3 - 3x = 0$

=> $x_1 = 0$ $\quad x_{2,3} = \mp\sqrt{\dfrac{3}{5}} = \mp 0.7745966$

$$w_1 = \frac{2\left(1 - 0^2\right)}{3^2\left[P_2(0)\right]^2} = \frac{2}{9\left[\frac{1}{2}\left(3.0^2 - 1\right)\right]^2} = \frac{8}{9} = 0.888889$$

$$w_2 = \frac{2\left(1 - 0.7745966^2\right)}{3^2\left[P_2(0.7745966)\right]^2} = \frac{2\left(1 - 0.7745966^2\right)}{9\left[\frac{1}{2}\left(3 * 0.7745966^2 - 1\right)\right]^2} = 0.555556$$

$$w_3 = w_2$$

Example: Find the Gauss quadratures for n=2.

$$P_2(x)=\frac{1}{2}\left(3x^2-1\right)=0 \qquad => \qquad x_{1,2}=\mp 0.577350$$

$$w_k=\frac{2\left(1-x_k^2\right)}{n^2\left[P_{n-1}(x_k)\right]^2}$$

$$w_1=\frac{2\left[1-\left(\frac{1}{\sqrt{3}}\right)^2\right]}{2^2\left[\frac{1}{\sqrt{3}}\right]^2}=1 \qquad \& \qquad w_2=w_1$$

----------oooooooooooo-----------

The error equation that occurs in the solutions made with the Gauss-Legendre formulas is as follows,

$$R_n=\frac{2^{2n+1}(n!)^4}{(2n+1)\left[(2n)!\right]^2}f^{(2n)}(c) \qquad , \qquad -1\le c\le 1$$

If the limits of the integral are not between -1 and 1, but between two different values such as a and b, the following formulas must be used to calculate the integral.

$$\int_a^b f(y)dy \cong \left(\frac{b-a}{2}\right)\sum_{i=1}^{n} w_i . f(y_i)+R_n \qquad *$$

$$y_i=\left(\frac{b-a}{2}\right)x_i+\left(\frac{b+a}{2}\right)$$

Error Function ; $R_n = \dfrac{(b-a)^{2n+1}(n!)^4}{(2n+1)[(2n)!]^3} f^{(2n)}(c)$

Example: Calculate the integral $\int_{-1}^{1} x^2 \cos(x)dx$ for $n=3$ by using Gauss-Legendre formulas.

$$P_3(x) = \frac{1}{2}\left(5x^3 - 3x\right) = 0 \quad => \quad 5x^3 - 3x = 0$$

$$=> \quad x_1 = 0 \quad \& \quad x_{2,3} = \mp\sqrt{\frac{3}{5}} = \mp 0.7745966$$

$$w_1 = \frac{2\left(1-0^2\right)}{3^2\left[P_2(0)\right]^2} = \frac{2}{9\left[\frac{1}{2}\left(3.0^2 - 1\right)\right]^2} = \frac{8}{9} = 0.888889$$

$$w_2 = \frac{2\left(1-0.7745966^2\right)}{3^2\left[P_2(0)\right]^2} = \frac{2\left(1-0.7745966^2\right)}{9\left[\frac{1}{2}\left(3*0.7745966^2 - 1\right)\right]^2} = 0.555556 \quad \& \quad w_3 = w_2$$

$$\int_{-1}^{1} x^2 \cos(x)dx \cong w_1.f(x_1) + w_2.f(x_2) + w_3.f(x_3)$$

$$\int_{-1}^{1} x^2 \cos(x)dx \cong 0.888889*(0) + 0.555556*\left((0.77459)^2 * \cos(0.77459)\right) + 0.555556*\left((-0.77459)^2 * \cos(-0.77459)\right)$$

$$\int_{-1}^{1} x^2 \cos(x)dx \cong 0.47650$$

Check by analytical solution;

$$\int_{-1}^{1} x^2 \cos(x)dx = 2x*\cos(x) - \left(x^2 - 2\right)*\sin(x)\Big|_{-1}^{1} = 0.47830$$

Example: Calculate the integral $\int_0^2 e^y dy$ for $n=3$ by using Gauss-Legendre formulas.

$$\int_0^2 e^y dy \cong \left(\frac{2-0}{2}\right)\sum_{i=1}^{3} w_i . f(y_i)$$

$$y_i = \left(\frac{b-a}{2}\right)x_i + \left(\frac{b+a}{2}\right) = x_i + 1$$

$$y_1 = x_1 + 1 = 0 + 1 = 1$$

$$y_2 = x_2 + 1 = 0.77459 + 1 = 1.77459$$

$$y_3 = x_3 + 1 = -0.77459 + 1 = 0.22541$$

=> $$\int_0^2 e^y dy \cong \left(\frac{2-0}{2}\right)\sum_{i=1}^{3} w_i . f(y_i) \cong 1\left[0.888889 * e^1 + 0.555556 * e^{1.77459} + 0.555556 * e^{0.22541}\right]$$

$$\int_0^2 e^y dy \cong 6.388853$$

Check by analytical solution; $\int_0^2 e^y dy = e^y \Big|_0^2 = e^2 - e^0 = 6.389056$

3.6) Gauss-Chebysev Integration Formula

$\int_{-1}^{1} \frac{f(x)}{\sqrt{1-x^2}}dx$, The integral has singular points in $x = \mp 1$. if we try to solve it with normal numerical methods, the integral goes to infinity at these points. In this case we use Chebysev formulas,

$$T_n(x) = \cos[n.(\arccos x_i)]$$

=> $$\int_{-1}^{1} \frac{f(x)}{\sqrt{1-x^2}}dx = \sum_{i=1}^{n} w_i * f(x_i) + R_n \quad , \quad w_i = \frac{\pi}{n}$$

We can calculate x_i such that

If $T_n(x) = \cos[n.(\arccos x_i)] = 0$,

$n * (\arccos x_i) = \frac{(2i-1)\pi}{2}$ becomes.

=> $$\arccos x_i = \frac{(2i-1)\pi}{2n}$$

$$\cos(\arccos x_i) = \cos\left(\frac{(2i-1)\pi}{2n}\right)$$

=> $$\boxed{x_i = \cos\left(\frac{(2i-1)\pi}{2n}\right)}$$

Error function, $R_n = \frac{\pi}{(2n)! * 2^{2n-1}} f^{(2n)}(c)$, $-1 \le c \le 1$

Example: Calculate the integral $\int_{-1}^{1} \frac{dx}{\sqrt{1-x^2}}$ for $n=3$ by using Gauss-Chebysev integration formula.

$$x_i = \cos\left[\frac{(2i-1)\pi}{2n}\right]$$

For $i=1$ $\qquad x_1 = \cos\left[\frac{(2*1-1)\pi}{2*3}\right] = \cos\left(\frac{\pi}{6}\right) = \frac{\sqrt{3}}{2}$

For $i=2$ $\qquad x_2 = \cos\left[\frac{(2*2-1)\pi}{2*3}\right] = \cos\left(\frac{\pi}{2}\right) = 0$

For $i=3$ $\qquad x_3 = \cos\left[\frac{(2*3-1)\pi}{2*3}\right] = \cos\left(\frac{5\pi}{6}\right) = -\frac{\sqrt{3}}{2}$

$$w_1 = w_2 = w_3 = \frac{\pi}{n} = \frac{\pi}{3}$$

where $f(x)=1$,

=> $$\int_{-1}^{1} \frac{dx}{\sqrt{1-x^2}} \cong w_1 * f(x_1) + w_2 * f(x_2) + w_3 * f(x_3)$$

$$\int_{-1}^{1} \frac{dx}{\sqrt{1-x^2}} \cong \frac{\pi}{3}(1+1+1) = \pi$$

Check by analytical solution ; $\qquad \int_{-1}^{1} \frac{dx}{\sqrt{1-x^2}} = \arcsin(x)\Big|_{-1}^{1} = \frac{\pi}{2} - \left(-\frac{\pi}{2}\right) = \pi$

Example: Calculate the integral $\int_{-1}^{1}\frac{x^4}{\sqrt{1-x^2}}dx$ for $n=3$ by using Gauss-Chebysev integration formula.

$$f(x)=x^4$$

$$x_i=\cos\left[\frac{(2i-1)\pi}{2n}\right]$$

For $i=1$ $\quad x_1=\cos\left[\frac{(2*1-1)\pi}{2*3}\right]=\cos\left(\frac{\pi}{6}\right)=\frac{\sqrt{3}}{2}$

For $i=2$ $\quad x_2=\cos\left[\frac{(2*2-1)\pi}{2*3}\right]=\cos\left(\frac{\pi}{2}\right)=0$

For $i=3$ $\quad x_3=\cos\left[\frac{(2*3-1)\pi}{2*3}\right]=\cos\left(\frac{5\pi}{6}\right)=-\frac{\sqrt{3}}{2}$

$$w_1=w_2=w_3=\frac{\pi}{n}=\frac{\pi}{3}$$

=> $\int_{-1}^{1}\frac{x^4dx}{\sqrt{1-x^2}}\cong w_1*f(x_1)+w_2*f(x_2)+w_3*f(x_3)$

$$\int_{-1}^{1}\frac{x^4dx}{\sqrt{1-x^2}}\cong\frac{\pi}{3}\left[\left(\frac{\sqrt{3}}{2}\right)^4+0^4+\left(-\frac{\sqrt{3}}{2}\right)^4\right]=\frac{3\pi}{8}$$

NOTE: If the limits of integral are between a and b, the formula becomes

$$\int_{a}^{b}\frac{f(y)}{\sqrt{(y-a)(b-y)}}dy=\left(\frac{b-a}{2}\right)\sum_{i=1}^{n}w_i*f(y_i)+R_n$$

$$y_i=\left(\frac{b-a}{2}\right)x_i+\left(\frac{b+a}{2}\right)$$

3.7) Gauss-Laguerre Formula

$$\int_0^\infty e^{-x} f(x)dx = \sum_{i=1}^{n} w_i * f(x_i) + R_n$$

Laguerre functions , $L_n(x) = e^x \dfrac{d^n}{dx^n}\left(e^{-x} x^n\right)$

Weighting function , $w_i = \dfrac{(n!)^2}{x_i\left[L_n'(x_i)\right]^2}$

Error function , $R_n = \dfrac{(n!)^2}{(2n)!} f^{(2n)}(c)$

Example: $\int_0^\infty e^{-x} \sin(x)dx = ?$

$$f(x) = \sin(x)$$

$$\int_0^\infty e^{-x} \sin(x)dx \cong \sum_{i=0}^{n} w_i * \sin(x_i)$$

n	2	6	10	14
$\sum_{i=0}^{n} w_i * \sin(x_i)$	0.43	0.50005	0.500002	0.500000

3.8) Gauss-Hermite Formula

$$\int_{-\infty}^{\infty} e^{-x^2} f(x)dx \cong \sum_{i=1}^{n} w_i * f(x_i) + R_n$$

Where x_i's are the roots of Hermite functions.

$$H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n}\left(e^{-x^2}\right)$$

$$w_i = \frac{2^{n+1} n! \sqrt{\pi}}{\left[H_n'(x_i)\right]^2} \qquad \text{and} \qquad R_n = \frac{n!\sqrt{\pi}}{2^n (2n)!} f^{(2n)}(c)$$

Example: $\int_{-\infty}^{\infty} e^{-x^2} \sin^2(x)dx = ?$

=> $$\int_{-\infty}^{\infty} e^{-x^2} \sin^2(x)dx = \sum_{i=1}^{n} w_i * \sin^2(x_i)$$

n	2	4	6	8	10
$\sum_{i=0}^{n} w_i * \sin^2(x_i)$	0.748	0.5655	0.560255	0.560202	0.560202

HOMEWORKS

1) $\int_0^1 x^x dx = ?$

2) $\int_0^{\pi} e^{\sin(x)} dx = ?$

3) $\int_0^{\infty} e^{-x} x^4 dx = ?$

4) $\int_0^{\infty} e^{-\left(x + \frac{1}{x}\right)} dx = ?$

5) $\int_{-\infty}^{\infty} e^{-x^2}\cos(x)dx = ?$

6) $\int_{-\infty}^{\infty} e^{-x^2-\frac{1}{x^2}}dx = ?$

7) $\int_{-1}^{1} \frac{\cos(x)}{\sqrt{1-x^2}}dx = ?$

8) $\int_{-1}^{1} \frac{\sqrt{1+x^2}}{\sqrt{1-x^2}}dx = ?$

3.9) Multiple Integrals

$$I = \int_{x=a}^{b}\int_{y=c}^{d} f(x,y).dy.dx$$

The integral can be separated two parts,

If we say $F(x) = \int_{y=c}^{d} f(x,y).dy$, then I integral becomes $I = \int_{x=a}^{b} F(x).dx$.

=> $$F(x) = \int_{y=c}^{d} f(x,y).dy \cong \left(\frac{d-c}{2}\right)\sum_{j=1}^{m} w_j * f(x, y_j)$$

$$y_j = \left(\frac{d-c}{2}\right)\bar{x}_j + \left(\frac{d+c}{2}\right)$$

=> $$I = \int_{x=a}^{b} F(x).dx \cong \int_{x=a}^{b}\left(\frac{d-c}{2}\right)\sum_{j=1}^{m} w_j * f(x, y_j).dx$$

$$I = \left(\frac{d-c}{2}\right)\left(\frac{b-a}{2}\right)\sum_{k=1}^{n} w_k\left(\sum_{j=1}^{m} w_j * f(x_k, y_j)\right)$$

$$x_k = \left(\frac{b-a}{2}\right)\bar{x}_k + \left(\frac{b+a}{2}\right)$$

$$I = \frac{(b-a)(d-c)}{4}\sum_{k=1}^{n}\left(\sum_{j=1}^{m} w_k * w_j * f(x_k, y_j)\right)$$

Example: $A=\int_{x=0}^{2}\int_{y=-1}^{1}\frac{dy.dx}{x^2+y^2}=?$ Find the approximate value of integral by dividing the integrals by x and y into two parts.

$$A=\int_{x=0}^{2}\int_{y=-1}^{1}\frac{dy.dx}{x^2+y^2}\cong\frac{(2-0)(1-(-1))}{4}\sum_{k=1}^{2}\sum_{j=1}^{2}w_k * w_j * \frac{1}{x_k^2+y_j^2}$$

$$x_k=\left(\frac{b-a}{2}\right)\bar{x}_k+\left(\frac{b+a}{2}\right)=\bar{x}_k+1$$

$$y_j=\bar{x}_j$$

If we assume $m=n=2$,

For integral depends on x,

$\bar{x}_1=0.57735$ => $x_1=\bar{x}_1+1=0.57735+1=1.57735$

$\bar{x}_2=-0.57735$ => $x_2=\bar{x}_2+1=-0.57735+1=0.42265$

$w_1=w_2=1$

For integral depends on y,

$\bar{x}_1=0.57735$ => $y_1=\bar{x}_1=0.57735$

$\bar{x}_2=-0.57735$ => $y_2=\bar{x}_2=-0.57735$

$w_1=w_2=1$

$$A=\int_{x=0}^{2}\int_{y=-1}^{1}\frac{dy.dx}{x^2+y^2}\cong\frac{(2-0)(1-(-1))}{4}\sum_{k=1}^{2}\sum_{j=1}^{2}w_k * w_j * \frac{1}{x_k^2+y_j^2}$$

$$A\cong\sum_{k=1}^{2}\left(\frac{1}{x_k^2+y_1^2}+\frac{1}{x_k^2+y_2^2}\right)\cong\left(\frac{1}{x_1^2+y_1^2}+\frac{1}{x_1^2+y_2^2}+\frac{1}{x_2^2+y_1^2}+\frac{1}{x_2^2+y_2^2}\right)$$

=> $A\cong 4.61538$

Example: $A=\int_0^1\int_0^x x.y.e^{-y^2}dy.dx=?$ Find the approximate value of integral by dividing the integrals by x and y into two parts.

$$A=\int_0^1 x\left\{\int_0^x y.e^{-y^2}dy\right\}dx$$

=> If $I(x)=\int_0^x y.e^{-y^2}dy$ then "*A*" integral becomes $A=\int_0^1 x.I(x)dx$

$$I(x)=\int_0^x y.e^{-y^2}dy=\left(\frac{b-a}{2}\right)\sum_{i=1}^{2}w_i * f(y_i)$$

$\bar{x}_{1,2}=\mp 0.57735$ and $w_1=w_2=1$

$y_i=\left(\frac{b-a}{2}\right)\bar{x}_i+\left(\frac{b+a}{2}\right)$ => $y_i=\left(\frac{x-0}{2}\right)\bar{x}_i+\left(\frac{x+0}{2}\right)=\left(\frac{x}{2}\right)\bar{x}_i+\frac{x}{2}$

$$y_1=\frac{x}{2}(0.57735)+\frac{x}{2}=0.788675x$$

$$y_2=\frac{x}{2}(-0.57735)+\frac{x}{2}=0.211325x$$

=> $I(x)=\frac{x}{2}\left[1*f(y_1)+1*f(y_2)\right]$

$$I(x)=\frac{x}{2}\left[(0.788675x)*e^{-(0.788675x)^2}+(0.211325x)*e^{-(0.211325x)^2}\right]$$

=> $A=\int_0^1\left\{0.394338.x^3.e^{-0.622.x^2}+0.105663.x^3.e^{-0.04466.x^2}\right\}dx$

$x_i=\left(\frac{b-a}{2}\right)\bar{x}_i+\left(\frac{b+a}{2}\right)$ => $x_i=\left(\frac{1-0}{2}\right)\bar{x}_i+\left(\frac{1+0}{2}\right)=\frac{\bar{x}_i}{2}+\frac{1}{2}$

$$x_1=\frac{0.57735}{2}+\frac{1}{2}=0.788675$$

$$x_2 = \frac{-0.57735}{2} + \frac{1}{2} = 0.211325$$

$$A = \left(\frac{b-a}{2}\right)\sum_{j=1}^{2} w_j * g\left(x_j\right)$$

=> $$A = \frac{1}{2}\left\{0.394338.\left(0.788675\right)^3.e^{-0.622*\left(0.788675\right)^2} + 0.105663.\left(0.788675\right)^3.e^{-0.04466*\left(0.788675\right)^2}\right\} +$$

$$\frac{1}{2}\left\{0.394338.\left(0.211325\right)^3.e^{-0.622*\left(0.211325\right)^2} + 0.105663.\left(0.211325\right)^3.e^{-0.04466*\left(0.211325\right)^2}\right\}$$

=> $$A = 0.0932$$

4) NUMERICAL DIFFERENTIAL

4.1) Forward and Backward Differences

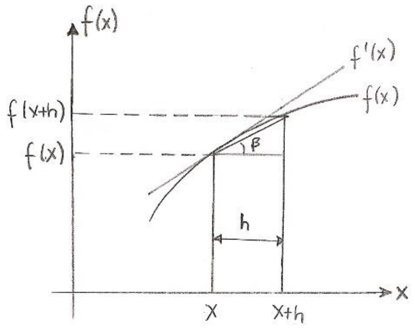
If we expand the $f(x)$ function to a Taylor series at a distance *h* from *x*, we get,

$$f(x+h) = f(x) + h.f'(x) + \frac{h^2}{2!} f''(x) + \frac{h^3}{3!} f'''(x) + \ldots$$

In this case $f'(x)$ can be obtained such that,

=> $$f'(x) = \frac{f(x+h) - f(x)}{h} - \frac{h}{2} f''(x) - \frac{h^2}{6} f'''(x) + \ldots$$

=> $$f'(x) = \frac{f(x+h) - f(x)}{h} + O(h)$$ ***(Forward Difference Formula)***



$f(x)$ => f_i

$f(x+h)$ => f_{i+1}

=> $$f_i' = \frac{f_{i+1} - f_i}{h} + O(h)$$ ***(Forward Difference Formula)***

If we repeat the above operations for a point at a negative distance of *h* from the selected point *x*, we get

$$f(x-h) = f(x) - h.f'(x) + \frac{h^2}{2!} f''(x) - \frac{h^3}{3!} f'''(x) + \ldots$$

$$f'(x) = \frac{f(x) - f(x-h)}{h} + \frac{h}{2} f''(x) - \frac{h^2}{6} f'''(x) + \ldots$$

=> $$f'(x) = \frac{f(x) - f(x-h)}{h} + O(h)$$

=> $$f_i' = \frac{f_i - f_{i-1}}{h} + O(h)$$ ***(Backward Difference Formula)***

Operators

$\Delta f_i = f_{i+1} - f_i$ => $f_i' = \frac{\Delta f_i}{h} + O(h)$ ***(Forward Difference Formula)***

$\nabla f_i = f_i - f_{i-1}$ => $f_i' = \frac{\nabla f_i}{h} + O(h)$ ***(Backward Difference Formula)***

In order to calculate the quadratic forward difference formula, the solution is obtained by opening the $f(x+h)$ and $f(x+2h)$ functions to the Taylor series.

2/ $$f(x+h) = f(x) + h.f'(x) + \frac{h^2}{2!} f''(x) + \frac{h^3}{3!} f'''(x) + \ldots$$

— $$f(x+2h) = f(x) + 2h.f'(x) + \frac{(2h)^2}{2!} f''(x) + \frac{(2h)^3}{3!} f'''(x) + \ldots$$

$$2f(x+h) - f(x+2h) = f(x) - h^2 f''(x) - h^3 f'''(x) - \ldots$$

=> $$f''(x) = \frac{f(x+2h) - 2f(x+h) + f(x)}{h^2} - hf'''(x) - \ldots$$

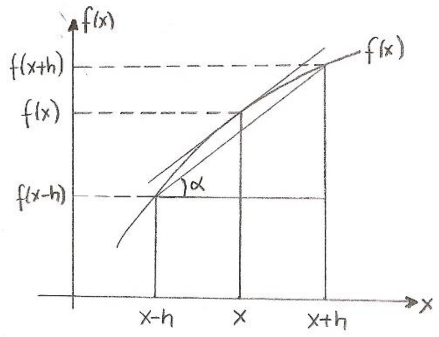
$$f_i'' = \frac{f_{i+2} - 2f_{i+1} + f_i}{h^2} + O(h)$$ ***(Quadratic Forward Difference Formula)***

$$f_i'' = \frac{f_i - 2f_{i-1} + f_{i-2}}{h^2} + O(h)$$ ***(Quadratic Backward Difference Formula)***

$$\Delta^2 f_i = f_{i+2} - 2f_{i+1} + f_i \quad => \quad f_i'' = \frac{\Delta^2 f_i}{h^2} + O(h)$$

$$\nabla^2 f_i = f_i - 2f_{i-1} + f_{i-2} \quad => \quad f_i'' = \frac{\nabla^2 f_i}{h^2} + O(h)$$

4.2) Central Differences



$$f'(x) \cong \frac{f(x+h) - f(x-h)}{2h} \cong \tan\alpha$$

$$f(x+h) = f(x) + h.f'(x) + \frac{h^2}{2!} f''(x) + \frac{h^3}{3!} f'''(x) + \ldots \qquad (1)$$

$$- \quad f(x-h) = f(x) - h.f'(x) + \frac{h^2}{2!} f''(x) - \frac{h^3}{3!} f'''(x) + \ldots \qquad (2)$$

$$f(x+h) - f(x-h) = 2h.f'(x) + \frac{2h^3}{3!} f'''(x) + \ldots$$

$$=> \quad f'(x) = \frac{f(x+h) - f(x-h)}{2h} - \frac{h^2}{6} f'''(x) - \ldots$$

=> $$f'(x)=\frac{f(x+h)-f(x-h)}{2h}+O(h^2)$$

If we add formulas (1) and (2) side by side,

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

=> $$f''(x)=\frac{f(x+h)-2f(x)+f(x-h)}{h^2}+O(h^2)$$

$$\left.\begin{aligned} f_i' &= \frac{f_{i+1}-f_{i-1}}{2h}+O(h^2) \\ f_i'' &= \frac{f_{i+1}-2f_i+f_{i-1}}{h^2}+O(h^2) \end{aligned}\right\}$$ ***Central Difference Formula***

4.3) Generalization of Difference Formulas

$$\left.\frac{d^n f}{dx^n}\right|_{x_j}=\frac{\Delta^n f_j}{h^n}+O(h)$$ ***Forward Difference Formula***

$$\left.\frac{d^n f}{dx^n}\right|_{x_j}=\frac{\nabla^n f_j}{h^n}+O(h)$$ ***Backward Difference Formula***

$$\left.\frac{d^n f}{dx^n}\right|_{x_j}=\frac{\nabla^n f_{j+\frac{n}{2}}+\Delta^n f_{j-\frac{n}{2}}}{2h^n}+O(h^2)$$, if n is even

Central Difference Formula

$$\left.\frac{d^n f}{dx^n}\right|_{x_j}=\frac{\nabla^n f_{j+\frac{(n-1)}{2}}+\Delta^n f_{j-\frac{(n-1)}{2}}}{2h^n}+O(h^2)$$, if n is odd

General Formulas,

$$\Delta^n f_j = \Delta^{n-1} f_{j+1} - \Delta^{n-1} f_j$$

$$\nabla^n f_j = \nabla^{n-1} f_j - \nabla^{n-1} f_{j-1}$$

Example: Calculate the central difference formula for $n = 2$.

$$\left.\frac{d^2 f}{dx^2}\right|_{x_j} = \frac{\nabla^2 f_{j+\frac{2}{2}} + \Delta^2 f_{j-\frac{2}{2}}}{2h^2} + O\left(h^2\right)$$

$$\left.\frac{d^2 f}{dx^2}\right|_{x_j} = \frac{\nabla^2 f_{j+1} + \Delta^2 f_{j-1}}{2h^2} + O\left(h^2\right) = \frac{\left(\nabla f_{j+1} - \nabla f_j\right) + \left(\Delta f_j - \Delta f_{j-1}\right)}{2h^2} + O\left(h^2\right)$$

$$\left.\frac{d^2 f}{dx^2}\right|_{x_j} = \frac{\left(f_{j+1} - f_j - f_j + f_{j-1}\right) + \left(f_{j+1} - f_j - f_j + f_{j-1}\right)}{2h^2} + O\left(h^2\right)$$

$$\left.\frac{d^2 f}{dx^2}\right|_{x_j} = \frac{\left(f_{j+1} - 2 f_j + f_{j-1}\right)}{h^2} + O\left(h^2\right)$$

Example:

x	0	1	2	3	4	5
$f(x)$	1	0.5	8.0	35.5	95	198.5

Find the third derivative of the function *f(x)* at $x = 0, 1, 2$ using the forward difference formulas.

Since the step interval is 1, it is taken as *h=1* in the expressions.

i	x_i	f_i	$\Delta f_i = f_{i+1} - f_i$	$\Delta^2 f_i = \Delta f_{i+1} - \Delta f_i$	$\Delta^3 f_i = \Delta^2 f_{i+1} - \Delta^2 f_i$
0	0	1	$0.5-1=-0.5$	$7.5-(-0.5)=8$	$20-8=12$
1	1	0.5	$8.0-0.5=7.5$	$27.5-7.5=20$	$32-20=12$
2	2	8.0	$35.5-8.0=27.5$	$59.5-27.5=32$	$44-32=12$
3	3	35.5	$95-35.5=59.5$	$103.5-59.5=44$	
4	4	95	$198.5-95=103.5$		
5	5	198.5			

$$\left.\frac{d^3 f}{dx^3}\right|_{x_j} = \frac{\Delta^3 f_j}{h^3} + O(h)$$

$h=1$ =>

$$\left.\frac{d^3 f}{dx^3}\right|_0 = \frac{\Delta^3 f_0}{1^3} = 12 \qquad \left.\frac{d^3 f}{dx^3}\right|_1 = \frac{\Delta^3 f_1}{1^3} = 12 \qquad \left.\frac{d^3 f}{dx^3}\right|_2 = \frac{\Delta^3 f_2}{1^3} = 12$$

4.4) Higher Order Forward, Backward, and Central Difference Formulas

If we write the forward difference formula,

$$f'(x) = \frac{f(x+h) - f(x)}{h} - \frac{h}{2} f''(x) - \frac{h^2}{6} f'''(x) + \ldots$$

When we write the second order forward difference formula instead of $f''(x)$ in this formula,

$$f''(x)=\frac{f(x+2h)-2f(x+h)+f(x)}{h^2}-hf'''(x)-\ldots$$

=> $$f'(x)=\frac{f(x+h)-f(x)}{h}-\frac{h}{2}\left[\frac{f(x+2h)-2f(x+h)+f(x)}{h^2}+O(h)\right]-\frac{h^2}{6}f'''(x)+\ldots$$

=> $$f'(x)=\frac{-f(x+2h)+4f(x+h)-3f(x)}{2h}+O(h^2)$$

$$\left.\begin{array}{ll} f_i'=\dfrac{-f_{i+2}+4f_{i+1}-3f_i}{2h}+O(h^2) & \text{Forward Difference} \\[2ex] f_i'=\dfrac{f_{i+1}-f_{i-1}}{2h}+O(h^2) & \text{Central Difference} \\[2ex] f_i'=\dfrac{f_{i-2}-4f_{i-1}+3f_i}{2h}+O(h^2) & \text{Backward Difference} \end{array}\right\}\ \textbf{(Three-Point Formulas)}$$

$$f_i'=\frac{f_{i-2}-8f_{i-1}+8f_{i+1}-f_{i+2}}{2h}+O(h^4)$$ **Central Difference (Five Point Formula)**

HOMEWORK

1)

x	0	0.5	1.0	1.5	2	2.5	3.0
$f(x)$	1	0.8	1.2	0.4	0.6	0.8	0.7

Solve by all approximations $f'(1.5)$ and $f'(1.5)$ so that the error order of $O(0.5^2)$

2) Obtain central difference formula for $f'''(x)$.

5) INTERPOLATION AND EXTRAPOLATION

5.1) Gregory-Newton Interpolation Formula

If the function $f(x)$ expand to Taylor series at $x=0$,

$$f(x)=f(0)+x.f'(0)+\frac{x^2}{2!}f''(0)+\frac{x^3}{3!}f'''(0)+\ldots$$

$$f'(0)=\frac{\Delta f_0}{h}-h.f'''(0)+O(h^2)$$

, by substituting forward difference expression in Taylor series, we obtain

$$f(x)=f(0)+\frac{x}{h}\Delta f_0+\frac{x(x-h)}{2!.h^2}\Delta^2 f_0+\frac{x(x-h)(x-2h)}{3!.h^3}\Delta^3 f_0+\ldots$$

If we expand it to the Taylor series at $x=x_n$, we can generalize the formula as

$$f(x)=f(x_n)+\frac{(x-x_n)}{h}\Delta f_n+\frac{(x-x_n)[(x-x_n)-h]}{2!.h^2}\Delta^2 f_n+\frac{(x-x_n)[(x-x_n)-h][(x-x_n)-2h]}{3!.h^3}\Delta^3 f_n+\ldots$$

(Gregory-Newton interpolation formula with forward difference)

If we repeat these steps with the backward difference formula,

$$f(x)=f(x_n)+\frac{(x-x_n)}{h}\nabla f_n+\frac{(x-x_n)[(x-x_n)+h]}{2!.h^2}\nabla^2 f_n+\frac{(x-x_n)[(x-x_n)+h][(x-x_n)+2h]}{3!.h^3}\nabla^3 f_n+\ldots$$

(Gregory-Newton interpolation formula with backward difference)

If the data are **equally spaced**, the Gregory-Newton interpolation formula is used to interpolate or extrapolate.

Example:

x	0	1	2	3	4	5
$f(x)$	-7	-3	6	25	62	129

Estimate the value of $f(1.1)$ based on the given values.

When we look at the values, since there are more points beyond the 1.1 point, the forward difference formula will be used.

$$f(x) = f(x_n) + \frac{(x-x_n)}{h}\Delta f_n + \frac{(x-x_n)[(x-x_n)-h]}{2!.h^2}\Delta^2 f_n + \frac{(x-x_n)[(x-x_n)-h][(x-x_n)-2h]}{3!.h^3}\Delta^3 f_n + \ldots$$

i	x_i	f_i	$\Delta f_i = f_{i+1} - f_i$	$\Delta^2 f_i = \Delta f_{i+1} - \Delta f_i$	$\Delta^3 f_i = \Delta^2 f_{i+1} - \Delta^2 f_i$
0	0	-7	$-3-(-7)=4$	$9-4=5$	$10-5=5$
1	1	-3	$6-(-3)=9$	$19-9=10$	$18-10=8$
2	2	6	$25-6=19$	$37-19=18$	$30-18=12$
3	3	25	$62-25=37$	$67-37=30$	-
4	4	62	$129-62=67$	-	-
5	5	129	-	-	-

i	x_i	f_i	$\Delta^4 f_i = \Delta^3 f_{i+1} - \Delta^3 f_i$	$\Delta^5 f_i = \Delta^4 f_{i+1} - \Delta^4 f_i$
0	0	-7	$8-5=3$	$4-3=1$
1	1	-3	$12-8=4$	-
2	2	6	-	-
3	3	25	-	-
4	4	62	-	-
5	5	129	-	-

Since the closest value to 1.1 is 1.0, $x_n = 1$ will be accepted. ($h = 1$ and $x = 1.1$)

$$f(x) = f(x_n) + \frac{(x - x_n)}{h}\Delta f_n + \frac{(x - x_n)[(x - x_n) - h]}{2!.h^2}\Delta^2 f_n + \frac{(x - x_n)[(x - x_n) - h][(x - x_n) - 2h]}{3!.h^3}\Delta^3 f_n + ...$$

$$f(1.1) = f(1) + \frac{(1.1 - 1)}{1}\Delta f_1 + \frac{(1.1 - 1)[(1.1 - 1) - 1]}{2!.1^2}\Delta^2 f_1 + \frac{0.1[(0.1) - 1][(0.1) - 2]}{3!.1^3}\Delta^3 f_1 +$$
$$\frac{0.1[(0.1) - 1][(0.1) - 2][(0.1) - 3]}{4!.1^4}\Delta^4 f_1$$

$$f(1.1) = -3 + 0.1 * 9 + \frac{0.1 * (-0.9)}{2}10 + \frac{0.1 * (-0.9) * (-1.9)}{6}8 + \frac{0.1 * (-0.9) * (-1.9)(-2.9)}{24}4$$

$$f(1.1) = -2.40465$$

If we consider only first to terms the result would be

$f(1.1) = -3 + 0.1 * 9 = -2.1$ *(Linear Interpolation)*

5.2) INTERPOLATION TO UNEVEN DATA (LAGRANGE POLYNOMIALS)

If we write nth order polynomial for x_j point,

$$P_j(x) = A_j(x - x_0)(x - x_1)(x - x_2).....(x - x_{j-1})(x - x_{j+1}).....(x - x_n)$$

$$P_j(x) = A_j \prod_{\substack{i=0 \\ i \neq j}}^{n} (x - x_i)$$

If we were to find the value of the polynomial for any point, x_k

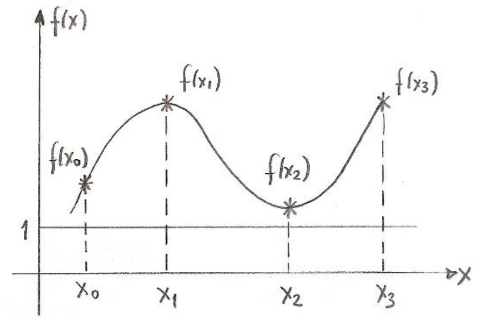
$$P_j(x_k) = \begin{cases} 0 & k \neq j \\ A_j \prod_{\substack{i=0 \\ i \neq j}}^{n} (x_j - x_i) & k = j \end{cases}$$

If $A_j = \dfrac{1}{\prod_{\substack{i=0 \\ i \neq j}}^{n} (x_j - x_i)}$ is chosen,

=> $P_j(x) = \dfrac{\prod_{\substack{i=0 \\ i \neq j}}^{n} (x - x_i)}{\prod_{\substack{i=0 \\ i \neq j}}^{n} (x_j - x_i)}$ ***(Lagrange Polynomials)***

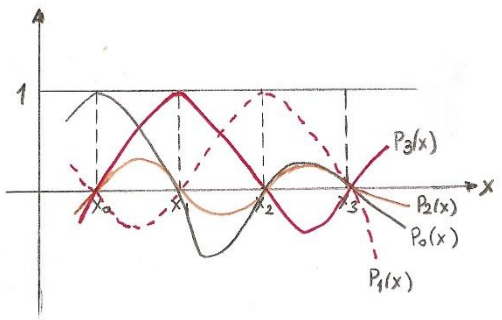
$$P_j(x_k) = \begin{cases} 0 & k \neq j \\ 1 & k = j \end{cases}$$

$$f(x) \cong \sum_{j=0} f(x_j) * P_j(x)$$



=> $$f(x) \approx f(x_0) * P_0(x) + f(x_1) * P_1(x) + f(x_2) * P_2(x) + f(x_3) * P_3(x)$$

=> $$P_0(x_k) = \begin{cases} 0 & k \neq 0 \\ 1 & k = 0 \end{cases}$$



=> $$f(x_0) = f(x_0) * 1 + f(x_1) * 0 + f(x_2) * 0 + f(x_3) * 0$$
$$f(x_1) = f(x_0) * 0 + f(x_1) * 1 + f(x_2) * 0 + f(x_3) * 0$$

Example:

i	0	1	2	3
x_i	1	2	4	8
$f(x_i)$	1	3	7	11

Find the Lagrangian function and calculate the value $f(7)$.

$$P_j(x) = \frac{\prod_{\substack{i=0 \\ i \neq j}}^{n} (x - x_i)}{\prod_{\substack{i=0 \\ i \neq j}}^{n} (x_j - x_i)}$$

=> $$P_0(x)=\frac{(x-x_1)(x-x_2)(x-x_3)}{(x_0-x_1)(x_0-x_2)(x_0-x_3)}=\frac{(x-2)(x-4)(x-8)}{(1-2)(1-4)(1-8)}$$

$$P_1(x)=\frac{(x-x_0)(x-x_2)(x-x_3)}{(x_1-x_0)(x_1-x_2)(x_1-x_3)}=\frac{(x-1)(x-4)(x-8)}{(2-1)(2-4)(2-8)}$$

$$P_2(x)=\frac{(x-x_0)(x-x_1)(x-x_3)}{(x_2-x_0)(x_2-x_1)(x_2-x_3)}=\frac{(x-1)(x-2)(x-8)}{(4-1)(4-2)(4-8)}$$

$$P_3(x)=\frac{(x-x_0)(x-x_1)(x-x_2)}{(x_3-x_0)(x_3-x_1)(x_3-x_2)}=\frac{(x-1)(x-2)(x-4)}{(8-1)(8-2)(8-4)}$$

=> $$f(x)=f(x_0)*P_0(x)+f(x_1)*P_1(x)+f(x_2)*P_2(x)+f(x_3)*P_3(x)$$

=> $$f(x)=1*P_0(x)+3*P_1(x)+7*P_2(x)+11*P_3(x)$$

=> $$f(7)=1*P_0(7)+3*P_1(7)+7*P_2(7)+11*P_3(7)$$

$$P_0(7)=\frac{(x-x_1)(x-x_2)(x-x_3)}{(x_0-x_1)(x_0-x_2)(x_0-x_3)}=\frac{(7-2)(7-4)(7-8)}{(1-2)(1-4)(1-8)}=\frac{5*3*-1}{-1*-3*-7}=0.71429$$

$$P_1(7)=\frac{(x-x_0)(x-x_2)(x-x_3)}{(x_1-x_0)(x_1-x_2)(x_1-x_3)}=\frac{(7-1)(7-4)(7-8)}{(2-1)(2-4)(2-8)}=\frac{6*3*-1}{1*-2*-6}=-1.5$$

$$P_2(7)=\frac{(x-x_0)(x-x_1)(x-x_3)}{(x_2-x_0)(x_2-x_1)(x_2-x_3)}=\frac{(7-1)(7-2)(7-8)}{(4-1)(4-2)(4-8)}=\frac{6*5*-1}{3*2*-4}=1.25$$

$$P_3(7)=\frac{(x-x_0)(x-x_1)(x-x_2)}{(x_3-x_0)(x_3-x_1)(x_3-x_2)}=\frac{(7-1)(7-2)(7-4)}{(8-1)(8-2)(8-4)}=\frac{6*5*3}{7*6*4}=0.53571$$

=> $$f(7)=1*0.71429+3*(-1.5)+7*1.25+11*0.53571$$

=> $$f(7)=10.8571$$

HOMEWORK

1)

i	0	1	2	3	4
x_i	2	4	6	7	9
$f(x_i)$	3	6	9	5	8

Find the Lagrange polynomial for the data given. Calculate the $f(8)$ and $f(1)$ values.

2)

i	0	1	2	3	4	5	6	7
x_i	0.1	0.3	0.7	0.9	1.2	1.5	1.7	2.0
$f(x_i)$	0.99	0.92	0.7	0.57	0.39	0.24	0.16	0.07

Find the Lagrange polynomial for the data given. Calculate the $f(1)$ value.

5.3) Extrapolation

If the function $f(x)$ is known only $a \le x \le b$ in the range, but the values of $f(x)$in $x < a$ or $x > b$ are desired, then extrapolation is performed. Gregory-Newton or Lagrange functions are used.

In order to be able to perform interpolation and extrapolation for $f(x)$, it must be suitable for polynomial interpolation.

Example:

x	1	2	3	4	5
$f(x)$	100	25	11.111	6.25	4

=> Find estimated value of $f(5.7)$.

Since the intervals are equal, we need to use the Gregory-Newton forward or backward difference formulas. Since the desired value is 5.7, we need to use the backward differences formula.

$$f(x) = f(x_n) + \frac{(x-x_n)}{h}\nabla f_n + \frac{(x-x_n)[(x-x_n)+h]}{2!.h^2}\nabla^2 f_n + \frac{(x-x_n)[(x-x_n)+h][(x-x_n)+2h]}{3!.h^3}\nabla^3 f_n + \ldots$$

(Gregory-Newton interpolation function with backward difference formula)

i	x_i	f_i	$\nabla f_i = f_i - f_{i-1}$	$\nabla^2 f_i = \nabla f_i - \nabla f_{i-1}$	$\nabla^3 f_i = \nabla^2 f_i - \nabla^2 f_{i-1}$	$\nabla^4 f_i = \nabla^3 f_i - \nabla^3 f_{i-1}$
0	1	100	-	-	-	-
1	2	25	-75	-	-	-
2	3	11.111	-13.889	61.111	-	-
3	4	6.25	-4.861	9.028	-52.083	-
4	5	4	-2.25	2.611	-6.417	45.666

$x_n = 5$ (closest to 5.7)

$x = 5.7$

$h = 1$

$$f(x) = f(x_n) + \frac{(x-x_n)}{h}\nabla f_n + \frac{(x-x_n)[(x-x_n)+h]}{2!.h^2}\nabla^2 f_n + \frac{(x-x_n)[(x-x_n)+h][(x-x_n)+2h]}{3!.h^3}\nabla^3 f_n + \ldots$$

$x - x_n = 5.7 - 5 = 0.7$

$$f(5.7) = f(5) + 0.7\nabla f_5 + \frac{0.7[0.7+1]}{2}\nabla^2 f_5 + \frac{0.7[1.7][2.7]}{6}\nabla^3 f_5 + \frac{0.7[1.7][2.7][3.7]}{24}\nabla^4 f_5$$

$$f(5.7) = 4 + 0.7*(-2.25) + \frac{0.7*1.7}{2}2.611 + \frac{0.7*1.7*2.7}{6}(-6.417) + \frac{0.7*1.7*2.7*3.7}{24}45.666$$

$$f(5.7) = 23.163$$

Not suitable for interpolation and extrapolation.

If we do linear interpolation taking the first two terms, we get

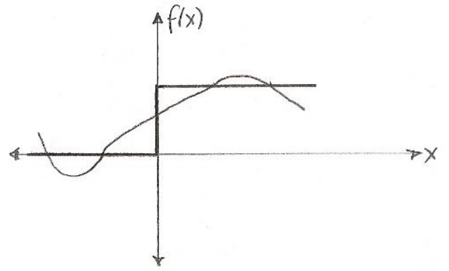
$$f(5.7) = f(5) + 0.7\nabla f_5 = 4 + 0.7*(-2.25) = 2.425$$

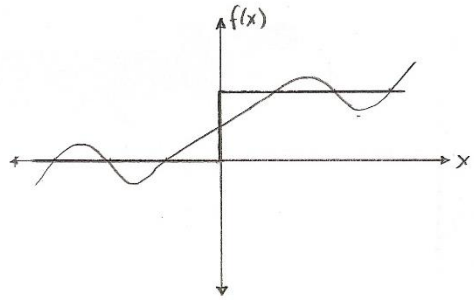
	Real Value $f(x) = \frac{100}{x^2}$	Linear	2. Degree	3. Degree	4. Degree
$f(5.7)$	3.078	2.425	3.979	0.543	23.163

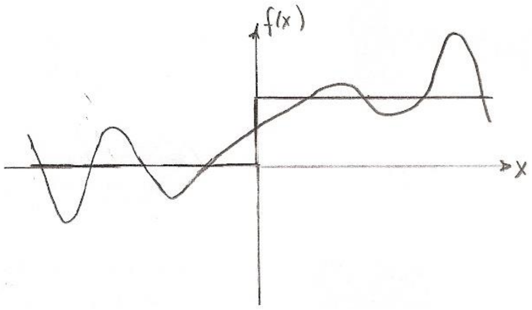
In such a case, the safest approach is the linear interpolation approach.

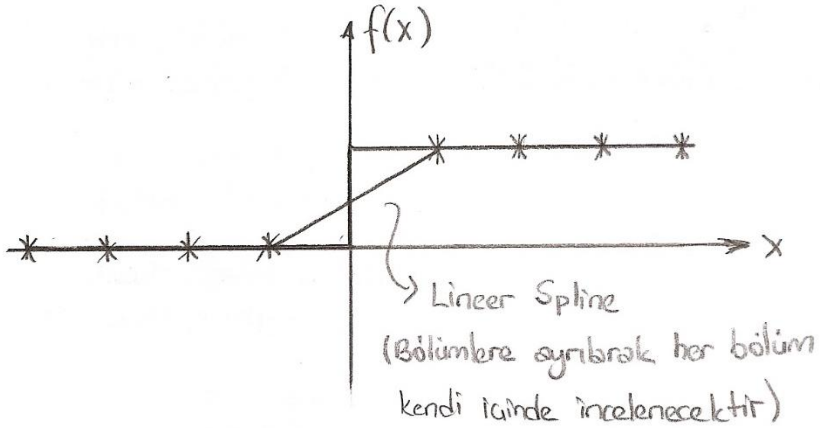
5.4) Spline Interpolation

In the interpolation methods we have examined under other headings, an n^{th} degree curve passes from the (n+1) points. However, passing high-order polynomials across data points could produce erroneous results when there were abrupt changes in data values. To avoid this, the data can be divided into smaller data groups and smaller order polynomial overlays can be made for each data group. Thus, the curve fitting operations made from small-order polynomials are called spline interpolation.


f(x)
x


f(x)
x


f(x)
x


f(x)
x
Lineer Spline
(Bölümlere ayrılarak her bölüm
kendi içinde incelenecektir)

Linear Spline

First-order spline functions for data groups given **in order** can be given as follows,

$$f(x) = f(x_0) + m_0(x - x_0) \qquad x_0 \le x \le x_1$$

$$f(x) = f(x_1) + m_1(x - x_1) \qquad x_1 \le x \le x_2$$

.

.

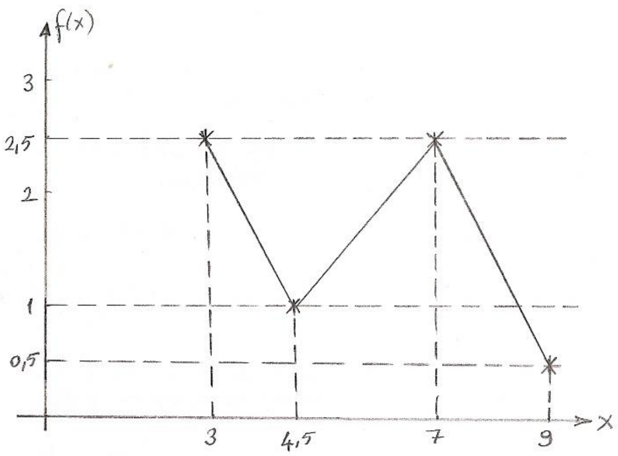
.

$$f(x) = f(x_{n-1}) + m_{n-1}(x - x_{n-1}) \qquad x_{n-1} \le x \le x_n$$

Here the slope expression, $m_i = \dfrac{f(x_{i+1}) - f(x_i)}{x_{i+1} - x_i}$

Example: For the data group given below, apply the linear spline and calculate $f(5)$.

i	0	1	2	3
x_i	3.0	4.5	7.0	9.0
$f(x_i)$	2.5	1.0	2.5	0.5



$$f(x) = f(x_1) + m_1(x - x_1) \qquad\qquad x_1 \le x \le x_2$$

$$f(x) = 1 + m_1(x - 4.5)$$

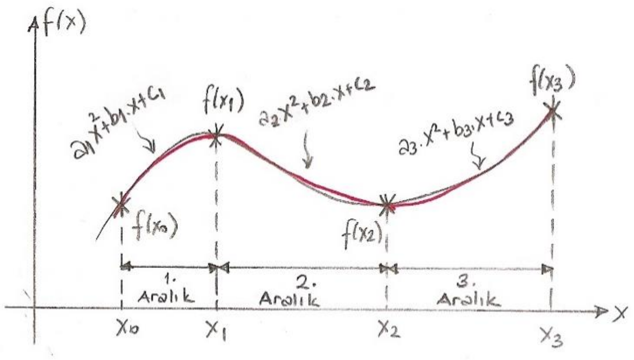
$$m_1 = \frac{f(x_2) - f(x_1)}{x_2 - x_1} = \frac{2.5 - 1}{7 - 4.5} = 0.6$$

$$f(x) = 1 + 0.6 * (x - 4.5) \qquad\qquad 4.5 \le x \le 7$$

=> $$f(5) = 1 + 0.6 * (5 - 4.5) = 1.3$$

Quadratic Spline

As seen in the example above, the curve at the node (data) points is discontinuous and 1., 2., …, n. derivatives are undefined. If it is required, the continuous mth derivative, It is necessary to pass a (m+1) degree polynomial. If a third-order polynomial is passed through the data points, both the 1st and 2nd derivatives are defined. For this reason, cubic splines are mostly used in spline interpolation. In a quadratic spline, the goal is to pass a second-order curve through the data points. As a result, the first derivative is defined at the data points.



$$f_i(x) = a_i.x^2 + b_i.x + c_i$$

For (n+1) data points, there are n intervals in total.

There are (3n) unknowns in total consisting of a's, b's and c's.

Then a total of (3n) conditions (equations) are needed. These;

i) At internal data points, the function values must be equal to the data values.

$$\left.\begin{aligned} a_{i-1}.x_{i-1}^2 + b_{i-1}.x_{i-1} + c_{i-1} &= f(x_{i-1}) \\ a_i.x_{i-1}^2 + b_i.x_{i-1} + c_i &= f(x_{i-1}) \end{aligned}\right\} \quad \{ i = 2, 3, ..., n$$

This condition satisfies 2(n-1) equation.

ii) First and last functions must pass through first and last data points.

$$a_1.x_0^2 + b_1.x_0 + c_1 = f(x_0)$$

$$a_n.x_n^2 + b_n.x_n + c_n = f(x_n)$$

This provides 2 equations.

iii) The first derivatives must be equal at the internal data points.

$$f'(x) = 2a.x + b$$

$$2a_{i-1}.x_{i-1} + b_{i-1} = 2a_i.x_{i-1} + b_i \qquad i = 2, 3, ..., n$$

This provides $(n-1)$ equations.

iv) At the first data point, the second derivative is **assumed** to be “0”.

$$2a_1 = 0 \qquad => \qquad a_1 = 0$$

In this case, the first function is a straight line, not a quadratic curve.

Example: For the data given in the previous example, solve the quadratic spline and calculate $f(5)$.

i	0	1	2	3
x_i	3.0	4.5	7.0	9.0
$f(x_i)$	2.5	1.0	2.5	0.5

Here n=3 and 3n=9 unknowns. If we write the 9 equations that depend on these 9 unknowns,

$$20,25a_1 + 4.5b_1 + c_1 = 1 \quad (1)$$

$$20,25a_2 + 4.5b_2 + c_2 = 1 \quad (2)$$

$$49a_2 + 7b_2 + c_2 = 2.5 \quad (3)$$

$$49a_3 + 7b_3 + c_3 = 2.5 \quad (4)$$

$$9a_1 + 3b_1 + c_1 = 2.5 \quad (5)$$

$$81a_3 + 9b_3 + c_3 = 0.5 \quad (6)$$

$$9a_1 + b_1 = 9a_2 + b_2 \quad (7)$$

$$14a_2 + b_2 = 14a_3 + b_3 \quad (8)$$

$$a_1 = 0 \quad (9)$$

If we solve these equations with the Gauss elimination method, the equation becomes as follows,

$$\begin{array}{cccccccc} b_1 & c_1 & a_2 & b_2 & c_2 & a_3 & b_3 & c_3 \\ \end{array}$$

$$\begin{bmatrix} 4.5 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 20.25 & 4.5 & 1 & 0 & 0 & 0 \\ 0 & 0 & 49 & 7 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 49 & 7 & 1 \\ 3 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 81 & 9 & 1 \\ 1 & 0 & -9 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 14 & 1 & 0 & -14 & -1 & 0 \end{bmatrix} \begin{bmatrix} b_1 \\ c_1 \\ a_2 \\ b_2 \\ c_2 \\ a_3 \\ b_3 \\ c_3 \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \\ 2.5 \\ 2.5 \\ 2.5 \\ 0.5 \\ 0 \\ 0 \end{bmatrix}$$

If a solution is made,

$a_1 = 0$ $\quad b_1 = -1$ $\quad c_1 = 5.5$

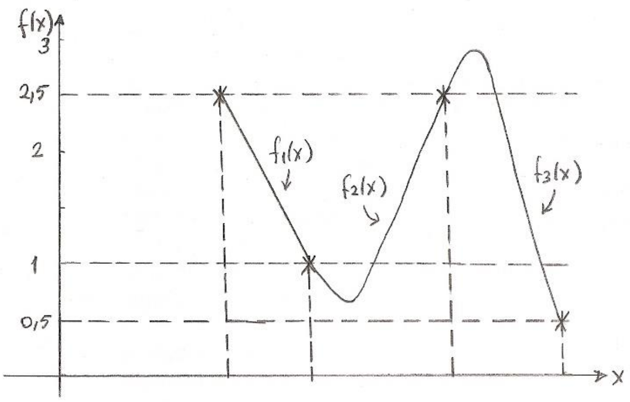
$a_2 = 0.64$ $\quad b_2 = -6.76$ $\quad c_2 = 18.46$

$a_3 = -1.6$ $\quad b_3 = 24.6$ $\quad c_3 = -91.3$

=> $f_1(x) = -x + 5.5 \qquad 3 \le x \le 4.5$

$f_2(x) = 0.64x^2 - 6.76x + 18.46 \qquad 4.5 \le x \le 7$

$f_3(x) = -1.6x^2 + 24.6x - 91.3 \qquad 7 \le x \le 9$



$x = 5$ => $f_2(5) = 0.64*25 - 6.76*5 + 18.46$

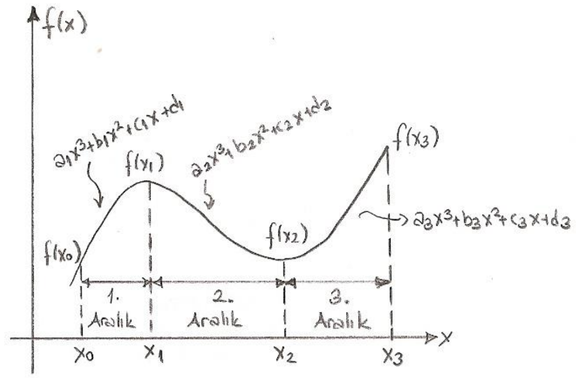
$f_2(5) = 0.66$

There are two important shortcomings in the quadratic spline solution;

i) The first two data points are joined with a straight line.
ii) Functions in both the first and last intervals show extreme oscillation.

The remedy for these weaknesses is the cubic spline. These deficiencies are not observed in the cubic spline.

Cubic Spline



=> $f_i(x)=a_i x^3+b_i x^2+c_i x+d_i$

For (n+1) data points,

There are n intervals.

4n unknowns appear (a, b, c, d's)

<u>Conditions:</u>

1) Function values at internal data points must be equal to the data value.
It provides 2(n-1) equations.

2) The first function must pass through the first data point, and the last function must pass through the last data point.
It provides 2 equations.

3) The value of the first derivatives of the functions at the internal data points must be equal.
It provides (n-1) equations.

4) The value of the second derivatives of the functions at the internal data points must be equal.
It provides (n-1) equations.

5) The second derivatives of the functions passing through the first and last data points must be "0". (Forcing Condition). It provides 2 equations.

In the sum of these items, 4n equations are obtained and a solution is made in this way.

Since the number of equations is too large during these operations, a set of equations has been developed for each region and generalized as;

$$f_i(x)=\frac{f''(x_{i-1})}{6(x_i-x_{i-1})}(x_i-x)^3+\frac{f''(x_{i-1})}{6(x_i-x_{i-1})}(x-x_{i-1})^3+\left[\frac{f(x_{i-1})}{(x_i-x_{i-1})}-\frac{f''(x_{i-1})(x_i-x_{i-1})}{6}\right](x_i-x)$$

$$+\left[\frac{f(x_i)}{(x_i-x_{i-1})}-\frac{f''(x_i)(x_i-x_{i-1})}{6}\right](x-x_{i-1}) \quad , \ i=1,2,3,......,n \qquad \text{(A)}$$

$$(x_i-x_{i-1})f''(x_{i-1})+2(x_{i+1}-x_{i-1})f''(x_i)+(x_{i+1}-x_i)f''(x_{i+1})=\frac{6}{(x_{i+1}-x_i)}[f(x_{i+1})-f(x_i)]$$

$$+\frac{6}{(x_i-x_{i-1})}[f(x_{i-1})-f(x_i)] \quad , \ i=1,2,3,......,n-1 \qquad \text{(B)}$$

First, equation B is solved. After obtaining f'' values at internal points, those can be substituted in equation A and for each interval a third order curve is obtained.

Example: Calculate the cubic spline curves using the data below and calculate f(5).

i	0	1	2	3
x_i	3.0	4.5	7.0	9.0
$f(x_i)$	2.5	1.0	2.5	0.5

=> If we say i=1 in equation B,

$$(x_1-x_0)f''(x_0)+2(x_2-x_0)f''(x_1)+(x_2-x_1)f''(x_2)=\frac{6}{(x_2-x_1)}[f(x_2)-f(x_1)]+\frac{6}{(x_1-x_0)}[f(x_0)-f(x_1)]$$

$$(4.5-3)f''(3)+2(7-3)f''(4.5)+(7-4.5)f''(7)=\frac{6}{(7-4.5)}[f(7)-f(4.5)]+\frac{6}{(4.5-3)}[f(3)-f(4.5)]$$

If we say i=2 in equation B,

$$(7-4.5)f''(4.5)+2(9-4.5)f''(7)+(9-7)f''(9)=\frac{6}{(9-7)}[f(9)-f(7)]+\frac{6}{(7-4.5)}[f(4.5)-f(7)]$$

$f''(3)$ and $f''(9)$ values are equal to zero from the 5th condition. In this case, the above equations take the form:

$8.f''(4.5)+2.5f''(7)=9.6$ if i=1

$2.5.f''(4.5)+9.f''(7)=-9.6$ if i=2

=> $f''(4.5)=1.67909$

$f''(7)=-1.53308$

<u>For the first interval;</u>

If equation A is solved by setting i=1;

$$f_1(x)=\frac{f''(3)}{6(4.5-3)}(4.5-x)^3+\frac{f''(4.5)}{6(4.5-3)}(x-3)^3+\left[\frac{2.5}{4.5-3}-\frac{f''(3)(4.5-3)}{6}\right](4.5-x)$$
$$+\left[\frac{1}{4.5-3}-\frac{f''(4.5)(4.5-3)}{6}\right](x-3) \quad , \; i=1$$

$$f_1(x)=1.86566(x-3)^3+1.66667(4.5-x)+0.246894(x-3)$$

<u>For the second interval;</u>

If equation A is solved by setting i=2;

$$f_2(x)=0.111939(7-x)^3-0.102205(x-4.5)^3-0.299621(7-x)+1.638783(x-4.5) \quad , \; i=2$$

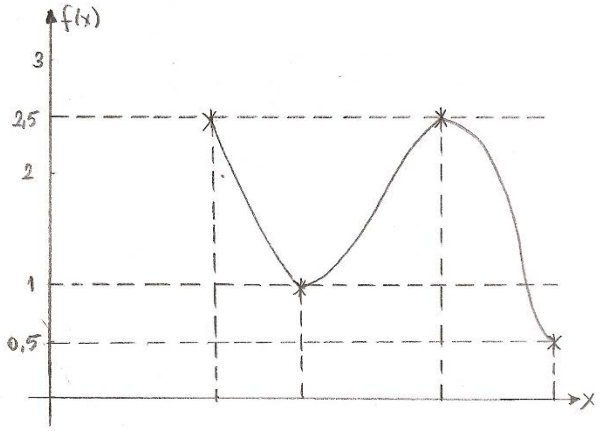
<u>For the third interval;</u>

If equation A is solved by setting i=3;

$$f_3(x) = -0.127757(9-x)^3 + 1.761027(9-x) + 0.25(x-7) \quad , \ i = 3$$

The point x=5 is valid for the second interval. In this situation,

$$f_2(5) = 1.102886$$



Cubic Interpolation

HOMEWORK

1) Construct quadratic and cubic splines for the data given below. Find the value of $f(0.47)$
.

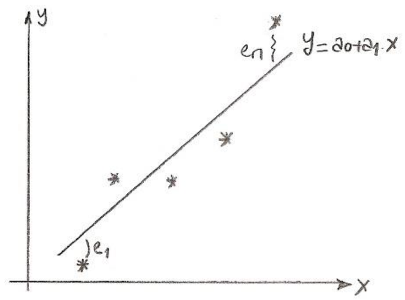
i	0	1	2	3	4	5	6	7	8
x_i	0	0.1	0.7	0.9	1.2	2.8	2.1	2.4	2.7
f_i	3.0	4.0	6.5	7.2	4.3	3.2	6.0	7.1	8.3

2) Write a computer program that overlaps a cubic spline with a curve.

LEAST SQUARE REGRESSION

If the data contains errors or is thought to contain errors, instead of the curve that will pass through all data points, the lower-order curve fitting that is thought to represent these data approximately and does not pass through all data points is called regression.

1. Linear Regression



$y = a_0 + a_1 x + e$, e ; error

$e = y - a_0 - a_1 x$

$e_i = y_i - a_0 - a_1 x_i$ (The difference between each point that makes up the function and the actual value gives the error value for that point.)

<u>Criterion for Optimal Curve</u>

The optimal curve is defined as the curve that minimizes the sum of the squared errors.

x_i	y_i
x_1	y_1
x_2	y_2
.	.
.	.
.	.
x_n	y_n

$$S_r = \sum_{i=1}^{n} e_i^2 = \sum_{i=1}^{n} \left(y_i - a_0 - a_1 x_i\right)^2$$

$$\frac{\partial S_r}{\partial a_0} = 0 \qquad => \qquad -2.\sum_{i=1}^{n} \left(y_i - a_0 - a_1 x_i\right) = 0 \qquad (1)$$

$$\frac{\partial S_r}{\partial a_1} = 0 \qquad => \qquad -2.\sum_{i=1}^{n} \left(y_i - a_0 - a_1 x_i\right) x_i = 0 \qquad (2)$$

(1) $\sum_{i=1}^{n} y_i - \sum_{i=1}^{n} a_0 - \sum_{i=1}^{n} a_1 x_i = 0$ => $\sum_{i=1}^{n} y_i = n.a_0 + \sum_{i=1}^{n} a_1 x_i$ (3)

(2) $\sum_{i=1}^{n} x_i.y_i - \sum_{i=1}^{n} a_0.x_i - \sum_{i=1}^{n} a_1 x_i^2 = 0$ => $\sum_{i=1}^{n} x_i.y_i = \sum_{i=1}^{n} x_i.a_0 + \sum_{i=1}^{n} x_i^2.a_1$ (4)

Example: Find the most appropriate linear line for the following data.

$n = 6$

i	x_i	y_i	$x_i.y_i$	x_i^2	y (result)
1	0.1	0.61	0.061	0.01	0.46262
2	0.4	0.92	0.368	0.16	0.99198
3	0.5	0.99	0.495	0.25	1.16844
4	0.7	1.52	1.064	0.49	1.52135
5	0.7	1.47	1.029	0.49	1.52135
6	0.9	2.03	1.827	0.81	1.87426
$\sum$	3.3	7.54	4.844	2.21	

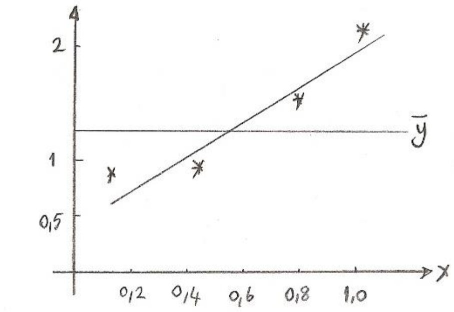
According to equation 3, $6a_0 + 3.3a_1 = 7.54$

According to equation 4, $3.3a_0 + 2.21a_1 = 4.844$

$a_1 = 1.7645$ and $a_0 = 0.2862$

$y = a_0 + a_1 x$

=> $y = 0.2862 + 1.7645x$



$$\bar{y} = \frac{\sum y_i}{n} = \frac{7.54}{6} = 1.25667$$

Determining the Amount of Error in Linear Regression:

a) Standard deviation of the regression line

$$S_{y/x} = \sqrt{\frac{S_r}{n-2}}$$

$S_{y/x}$: Standard deviation

$n-2$: Degrees of freedom

b) Coefficient of determination

$$r^2 = \frac{S_t - S_r}{S_t}$$

$$S_r = \sum_{i=1}^{n} e_i^2$$

$$S_t = \sum_{i=1}^{n} (y_i - \bar{y})^2 = \sum o_i^2$$

S_t, is the sum of the squares of the difference from the mean value of the dependent variable. Here, r is defined as the correlation coefficient.

In case of perfect curve overlap, r=0.

$$r^2 = r = 1 \qquad r^2 = \frac{S_t - 0}{S_t}$$

If $S_t = S_r$ then $r^2 = r = 0$, it means the curve did not provide any improvement.

If we calculate the amount of error for the previous example,

	$(y_i - a_0 - a_1 x_i)^2 = e_i^2$	$o_i^2 = (y_i - \bar{y})^2$
	0.02172	0.4181
	0.00518	0.1133
	0.03183	0.07111
	0.000001822	0.06931
	0.0026368	0.0455
	0.02425	0.598
$\sum$	0.08562	1.3153

$S_r = \sum e_i^2 = 0.08562$ and $S_t = \sum o_i^2 = 1.3153$

$$S_{y/x} = \sqrt{\frac{S_r}{n-2}} = \sqrt{\frac{0.08562}{6-2}} = 0.14630 \text{ (standard error)}$$

$$r^2 = \frac{S_t - S_r}{S_t} = \frac{1.3153 - 0.08562}{1.3153} = 0.935$$

=> $r = 0.9669$

2. Polynomial Regression

It may be more appropriate to represent the same data as a polynomial rather than a straight line. In this case, the least squares method can be applied similarly for the m[th] degree polynomial.

$$y = a_0 + a_1.x + a_2.x^2 + ... + a_m.x^m + e$$

$$e_i = y_i - a_0 - a_1.x_i - a_2.x_i^2 - ...... - a_m.x_i^m$$

$$S_r = \sum e_i^2 = \sum \left(y_i - a_0 - a_1.x_i - a_2.x_i^2 - ...... - a_m.x_i^m \right)^2$$

(1) $\dfrac{\partial S_r}{\partial a_0} = -2\sum \left(y_i - a_0 - a_1.x_i - a_2.x_i^2 - ...... - a_m.x_i^m \right) = 0$

(2) $\dfrac{\partial S_r}{\partial a_1} = -2\sum \left(y_i - a_0 - a_1.x_i - a_2.x_i^2 - ...... - a_m.x_i^m \right).x_i = 0$

.

.

(m+1) $\dfrac{\partial S_r}{\partial a_m} = -2\sum \left(y_i - a_0 - a_1.x_i - a_2.x_i^2 - ...... - a_m.x_i^m \right).x_i^m = 0$

1) $a_0 n + a_1 \sum x_i + a_2 \sum x_i^2 + ... + a_m \sum x_i^m = \sum y_i$

2) $a_0 \sum x_i + a_1 \sum x_i^2 + a_2 \sum x_i^3 + ... + a_m \sum x_i^{m+1} = \sum x_i y_i$

.

.

.

m+1) $a_0 \sum x_i^m + a_1 \sum x_i^{m+1} + a_2 \sum x_i^{m+2} + ... + a_m \sum x_i^{2m} = \sum x_i^m y_i$

Standard deviation,

$$S_{y/x} = \sqrt{\frac{S_r}{n - (m+1)}}$$

Coefficient of determination,

$$r^2 = \frac{S_t - S_r}{S_t}$$

Example: Calculate the 2nd order regression curve for the values given in the previous example?

$n = 6$

i	x_i	y_i	$x_i.y_i$	x_i^2
1	0.1	0.61	0.061	0.01
2	0.4	0.92	0.368	0.16
3	0.5	0.99	0.495	0.25
4	0.7	1.52	1.064	0.49
5	0.7	1.47	1.029	0.49
6	0.9	2.03	1.827	0.81
$\sum$	3.3	7.54	4.844	2.21

$$y = a_0 + a_1.x + a_2.x^2 + e$$

=> $e_i = y - a_0 - a_1.x_i - a_2.x_i^2$

$$S_r = \sum e_i^2 = \sum \left(y - a_0 - a_1.x_i - a_2.x_i^2\right)^2$$

$$\frac{\partial S_r}{\partial a_0} = 0 \quad => \quad -2\sum \left(y - a_0 - a_1.x_i - a_2.x_i^2\right) = 0 \qquad (1)$$

$$\frac{\partial S_r}{\partial a_1} = 0 \quad => \quad -2\sum \left(y - a_0 - a_1.x_i - a_2.x_i^2\right)x_i = 0 \qquad (2)$$

$$\frac{\partial S_r}{\partial a_2} = 0 \quad => \quad -2\sum \left(y - a_0 - a_1.x_i - a_2.x_i^2\right)x_i^2 = 0 \qquad (3)$$

1) $na_0 + a_1 \sum x_i + a_2 \sum x_i^2 = \sum y_i$ => $6a_0 + 3.3a_1 + 2.21a_2 = 7.54$

2) $a_0 \sum x_i + a_1 \sum x_i^2 + a_2 \sum x_i^3 = \sum x_i y_i$ => $3.3a_0 + 2.21a_1 + 1.605a_2 = 4.844$

3) $a_0 \sum x_i^2 + a_1 \sum x_i^3 + a_2 \sum x_i^4 = \sum x_i^2 y_i$ => $2.21a_0 + 1.605a_1 + 1.2245a_2 = 3.5102$

$a_0 = 0.587114$

$a_1 = 0.059102$

$a_2 = 1.729537$

$y = 0.587114 + 0.059102 .x + 1.729537 .x^2$ 2. degree regression polynomial

$y = 0.2862 + 1.7645x$ Linear regression polynomial

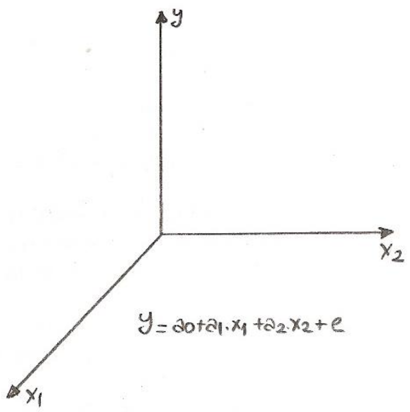
NOTE: Calculate correlation coefficient. Compare result with the linear regression result. Probably here r=0.98.

3. Multiple Linear Regression

If there is more than one variable. (assuming there are 2 variables)

x_{1i}	x_{2i}	y_i
.	.	.
.	.	.
.	.	.

In this case, not the best curve, but the plane that best represents the data will be found.



$e_i = y_i - a_0 - a_1 x_{1i} - a_2 x_{2i}$

$S_r = \sum e_i^2 = \sum \left(y_i - a_0 - a_1 x_{1i} - a_2 x_{2i} \right)^2$

$$\frac{\partial S_r}{\partial a_0} = 0 = -2\sum\left(y_i - a_0 - a_1 x_{1i} - a_2 x_{2i}\right) \quad => \quad n.a_0 + \sum x_{1i} a_1 + \sum x_{2i} a_2 = \sum y_i$$

$$\frac{\partial S_r}{\partial a_1} = 0 = -2\sum\left(y_i - a_0 - a_1 x_{1i} - a_2 x_{2i}\right).x_{1i} \quad => \quad \sum x_{1i} a_0 + \sum x_{1i}^2 a_1 + \sum x_{1i}.x_{2i}.a_2 = \sum x_{1i}.y_i$$

$$\frac{\partial S_r}{\partial a_2} = 0 = -2\sum\left(y_i - a_0 - a_1 x_{1i} - a_2 x_{2i}\right).x_{2i} \quad => \quad \sum x_{2i} a_0 + \sum x_{1i} x_{2i} a_1 + \sum x_{2i}^2.a_2 = \sum x_{2i}.y_i$$

HOMEWORK

1) Using the least squares regression method, find the first (linear), second, and third order polynomials for the data set given below. Compute and compare the coefficient of correlation for each case.

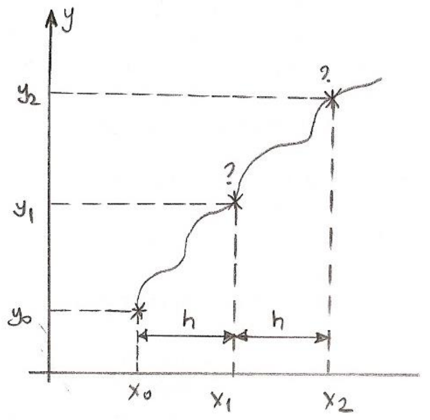
x_i	0	0.1	0.2	0.4	0.5	0.7	0.8	1.0
y_i	0	1.3	2.0	2.4	2.8	2.7	2.4	2.1

2) Using the least squares regression method, write a computer program that superimposes a 3rd degree polynomial curve and apply it to the above data.

6) NUMERICAL SOLUTION OF ORDINARY DIFFERENTIAL EQUATIONS

6.1.1) Numerical Solution of Initial Value Problems

$y' = f(x, y)$ and $y(x_0) = y_0$



$y_0 = y(x_0)$

$y_1 = y(x_0 + h)$

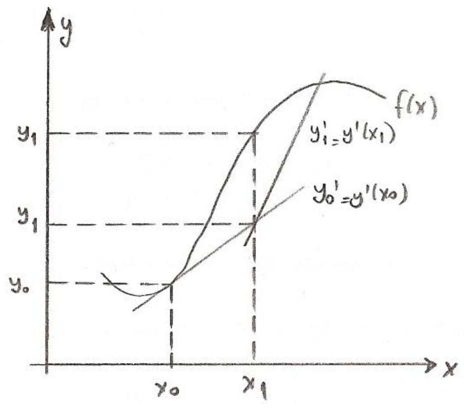
$y_2 = y(x_0 + 2h)$

.

.

.

$y_n = y(x_0 + nh)$



$$y_1 = y_0 + y'(x_0)(x_1 - x_0)$$

$$y_2 = y_1 + y'(x_1)(x_2 - x_1)$$

.

.

.

$$y_{n+1} = y_n + y'(x_n)(x_{n+1} - x_n)$$

=> $$y_{n+1} = y_n + y'(x_n)h$$

$$y'(x_n) = f(x_n, y_n)$$

$$y_{n+1} = y_n + h.f(x_n, y_n) + O(h^2)$$

This method is called the Euler method or the tangent line method.

6.1.2) Three-term Taylor Series Method

In the $y' = f(x, y)$ differential equation, if the initial value $y(x_0) = y_0$ is known, if we expand $y(x+h)$ to the Taylor series, we get,

$$y(x+h) = y(x) + y'(x).h + y''(x)\frac{h^2}{2!} + y'''(x)\frac{h^3}{3!} + ...$$

If we take first three term in Taylor series and apply chain rule to $y'(x)$ and $y''(x)$

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

$$y''(x) = \frac{\partial f[x, y(x)]}{\partial x}.\frac{dx}{dx} + \frac{\partial f[x, y(x)]}{\partial y}.\frac{dy}{dx}$$

=> $$y''(x) = \frac{\partial f[x, y(x)]}{\partial x} + \frac{\partial f[x, y(x)]}{\partial y} f[x, y(x)]$$

$$y(x+h)=y(x)+h.f[x,y(x)]+\frac{h^2}{2}\left\{\frac{\partial f[x,y(x)]}{\partial x}+\frac{\partial f[x,y(x)]}{\partial y}f[x,y(x)]\right\}+O(h^3)$$

$$y_{n+1}=y_n+h.f[x,y(x)]+\frac{h^2}{2}\left\{\frac{\partial f[x_n,y_n]}{\partial x}+\frac{\partial f[x_n,y_n]}{\partial y}f[x_n,y_n]\right\}+O(h^3)$$

Example: Numerically solve the differential equation given as $y'=x+y$ and $y(1)=-2$ compare the solution with the analytical solution results.

Analytical solution: $y=-x-1$

$f(x,y)=x+y$, $\frac{\partial f}{\partial x}=1$, $\frac{\partial f}{\partial y}=1$

=> $y_{n+1}=y_n+h.f[x_n,y_n]+\frac{h^2}{2}\{1+1(x_n+y_n)\}+O(h^3)$

If we choose $h=0.1$,

$x_n=x_0+nh$ => $x_n=1+0.1*n$

n	x_n	y_n (Analytical)	y_n (Numerical)
0	1	-2.0	-2.0
1	1.1	-2.1	-2.1
2	1.2	-2.2	-2.2
3	1.3	-2.3	-2.3
. .	. .	. .	. .
10	1.8	-2.8	-2.8

=> $y_{1,1}=y_1+0.1(1-2)+\frac{(0.1)^2}{2}\{1+1(1-2)\}+O(h^3)$

$y_{1,1}=-2.0-0.1=-2.1$

Example: $y' = y.\sin(x^2) - \cos(x^2) + 2y$, $y(3) = \sqrt{2}$

$$f(x,y) = y.\sin(x^2) - \cos(x^2) + 2y$$

$$\frac{\partial f}{\partial x} = 2xy.\cos(x^2) + 2x.\sin(x^2)$$

$$\frac{\partial f}{\partial y} = \sin(x^2) + 2$$

$$y_{n+1} = y_n + h.\left(y.\sin(x^2) - \cos(x^2) + 2y\right)_n + \frac{h^2}{2}\left\{2xy.\cos(x^2) + 2x.\sin(x^2) + \left(\sin(x^2) + 2\right)\left(y.\sin(x^2) - \cos(x^2) + 2y\right)\right\}_n + O(h^3)$$

If we choose $h = 0.1$,

$x_n = x_0 + nh$ => $x_n = 3 + 0.1 * n$

n	x_n	y_n
0	3.0	$\sqrt{2} = 1.4142$
1	3.1	1.7138
2	3.2	1.9156
3	3.3	1.9787
4	3.4	1.9512
5	3.5	1.9238
6	3.6	2.0176
. . .	. . .	. . .
10	4	4.0834

6.1.3) Runge-Kutta Method

$y'(x) = f(x, y)$ and $y(x_0) = y_0$

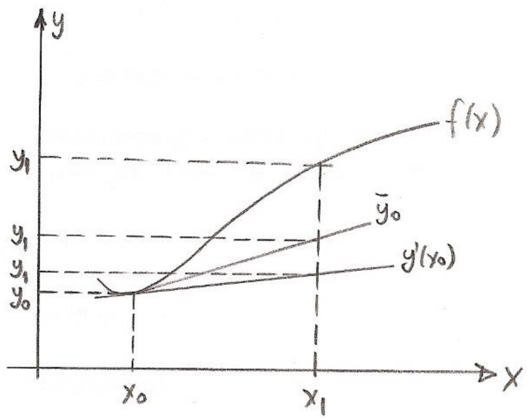
$$A_n = h.f(x_n, y_n)$$

$$B_n = h.f\left(x_n + \frac{1}{2}h, y_n + \frac{1}{2}A_n\right)$$

$$C_n = h.f\left(x_n + \frac{1}{2}h, y_n + \frac{1}{2}B_n\right)$$

$$D_n = h.f(x_n + h, y_n + C_n)$$

$$y_{n+1} = y_n + \frac{1}{6}[A_n + 2.B_n + 2.C_n + D_n] + O(h^5)$$



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

$$y_{n+1} = y_n + h.y'(x_n)$$

It is a very reliable method. The degree of error is extremely low and there is no problem of derivation.

Example: Solve the differential equation given by $y' = x^2 - \sin(y^2)$ and $y(1) = 4.7$

If we choose $h = 0.1$,

$f(x, y) = x^2 - \sin(y^2)$ $\qquad x_0 = 1 \qquad y_0 = 4.7$

$$A_0 = 0.1\{f(x_0, y_0)\} = 0.1 * \left[1^2 - \sin(4.7^2)\right] = 0.1099$$

$$B_0 = 0.1\left\{\left(1 + \frac{0.1}{2}\right)^2 - \sin\left(4.7 + \frac{0.1099}{2}\right)^2\right\} = 0.1682$$

$$C_0 = 0.1\left\{\left(1 + \frac{0.1}{2}\right)^2 - \sin\left(4.7 + \frac{0.1682}{2}\right)^2\right\} = 0.1884$$

$$D_0 = 0.1\left\{(1 + 0.1)^2 - \sin(4.7 + 0.1884)^2\right\} = 0.2115$$

$$y_1 = y_0 + \frac{1}{6}\left[A_0 + 2.B_0 + 2.C_0 + D_0\right] + O(h^5) = 4.7 + \frac{1}{6}\left[0.1099 + 2 * 0.1682 + 2 * 0.1884 + 0.2155\right]$$

=> $\quad y_1 = 4.8731$

$x_n = x_0 + nh$

$x_n = 1 + 0.1 * n$

$x = 1.1$, $y_1 = 4.8731$

n	x_n	y_n
0	1.0	4.7 (given)
1	1.1	4.8731
2	1.2	5.0426
3	1.3	5.1313
4	1.4	5.2168
5	1.5	5.4039
6	1.6	5.6797
7	1.7	5.8708

6.2) NUMERICAL SOLUTION OF SECOND DEGREE INITIAL VALUE PROBLEMS

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

6.2.1) Taylor Method

If we expand $y(x)$ to Taylor series at $x + h$,

$$y(x+h) = y(x) + y'(x).h + y''(x)\frac{h^2}{2!} + y'''(x)\frac{h^3}{3!} + ...$$

and

$$y'(x+h) = y'(x) + y''(x).h + y'''(x)\frac{h^2}{2!} + y^{(4)}(x)\frac{h^3}{3!} + ...$$

$$y(x+h) \cong y(x) + h.y'(x) + \frac{h^2}{2!}y''(x) + O(h^3)$$

$$y'(x+h) \cong y'(x) + h.y''(x) + O(h^2)$$

=> $\qquad y''_j = f(x_j, y_j, y'_j)$

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

$$y_{j+1} = y_j + h.y'_j + \frac{h^2}{2!}y''_j + O(h^3)$$

$$y'_{j+1} = y'_j + h.y''_j + O(h^2)$$

First we will take $j = 0$, and calculate y''_0, y_1 and y'_1. Then take $j = 1$ and calculate y''_1, y_2 and y'_2. By continuing the iteration process, y_1, y_2, y_3, ..., y_n will be obtained

Example: Solve the differential equation given by $y'' = x^2 - \cos(y) + 2.e^{-x}.y'$ with initial conditions $y(1) = -1$ and $y'(1) = 3$

$x_0 = 1 \qquad y_0 = -1 \qquad y'_0 = 3 \qquad f(x, y, y') = x^2 - \cos(y) + 2.e^{-x}.y'$

If $h = 0.1$ is chosen.

<u>Step 1:</u> $j = 0$

$$y''_0 = 1^2 - \cos(-1) + 2.e^{-1}.3 = 2.666974$$
$$x_1 = x_0 + 0.1*1 = 1.1$$
$$y_1 = -1 + 0.1*3 + \frac{(0.1)^2}{2} 2.666974 = -0.686665$$
$$y'_1 = 3 + 0.1*2.666974 = 3.2666974$$

<u>Step 2:</u> $j = 1$

$$y''_1 = 1.1^2 - \cos(-0.686665) + 2.e^{-1.1} * (3.266974) = 2.611405$$
$$x_2 = x_1 + 0.1*1 = 1.2$$
$$y_2 = -0.686665 + 0.1*3.2666974 + \frac{(0.1)^2}{2} 2.611405 = -0.346938$$
$$y'_2 = 3.2666974 + 0.1*2.611405 = 3.527838$$

<u>Step 3:</u> $j = 2$

$$y_3 = y(1.3) = 0.018939$$

6.2.2) Runge-Kutta Method

$y'' = f_2(x, y, y')$ $\qquad$ $y(x_0) = y_0$ $\qquad$ $y'(x_0) = P_0$

$y' = p = f_1(x, y, p)$ $\qquad$ => $\qquad$ $y(x_0) = y_0$

$y'' = p' = f_2(x, y, p)$ $\qquad$ => $\qquad$ $p(x_0) = P_0$

If $\qquad$ $y' = p + x = f_1(x, y, p)$ then

$p' + 1 = f_2(x, y, p)$ is obtained

$$k_1 = h.f_1(x_n, y_n, p_n)$$

$$l_1 = h.f_2(x_n, y_n, p_n)$$

$$k_2 = h.f_1\left(x_n + \frac{1}{2}h, y_n + \frac{1}{2}k_1, p_n + \frac{1}{2}l_1\right)$$

$$l_2 = h.f_2\left(x_n + \frac{1}{2}h, y_n + \frac{1}{2}k_1, p_n + \frac{1}{2}l_1\right)$$

$$k_3 = h.f_1\left(x_n + \frac{1}{2}h, y_n + \frac{1}{2}k_2, p_n + \frac{1}{2}l_2\right)$$

$$l_3 = h.f_2\left(x_n + \frac{1}{2}h, y_n + \frac{1}{2}k_2, p_n + \frac{1}{2}l_2\right)$$

$$k_4 = h.f_1(x_n + h, y_n + k_3, p_n + l_3)$$

$$l_4 = h.f_2(x_n + h, y_n + k_3, p_n + l_3)$$

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

$$p_{n+1} = p_n + \frac{1}{6}(l_1 + 2.l_2 + 2.l_3 + l_4)$$

Example: Solve the differential equation given by $x^2.y'' + 5.x.y' + 20.y = 0$ with initial conditions $y(1) = 0$ and $y'(1) = 2$. Evaluate $y(1.2) = ?$

=> $$y'' = -\frac{5.y'}{x} - \frac{20}{x^2}y$$

If $y' = p = f_1(x, y, p)$ is assumed

$$p' = -\frac{5}{x}p - \frac{20}{x^2}y = f_2(x, y, p)$$

$$y_0 = y(1) = 0$$

$$p_0 = p(1) = 2$$

If $h = 0.2$ is chosen,

$$k_1 = 0.2 * 2 = 0.4$$

$$l_1 = 0.2 * \left(-\frac{5}{1}2 - \frac{20}{1^2}0\right) = -2$$

$$k_2 = 0.2\left\{p_0 + \frac{1}{2}l_1\right\} = 0.2\left\{2 + \frac{1}{2}(-2)\right\} = 0.2$$

$$l_2 = 0.2\left\{\frac{-5}{1+\frac{0.2}{2}}\left(2 + \frac{-2}{2}\right) - \frac{20}{\left(1+\frac{0.2}{2}\right)^2}\left(0 + \frac{0.4}{2}\right)\right\} = -1.570$$

$$k_3 = 0.2\left\{2 + \frac{1}{2}(-1.57)\right\} = 0.243$$

$$l_3 = 0.2\left\{\frac{-5}{1+\frac{0.2}{2}}\left(2 + \frac{-1.57}{2}\right) - \frac{20}{\left(1+\frac{0.2}{2}\right)^2}\left(0 + \frac{0.2}{2}\right)\right\} = -1.435$$

$$k_4 = 0.2\{2 + (-1.435)\} = 0.113$$

$$l_4 = 0.2\left\{\frac{-5}{1+0.2}(2 - 1.435) - \frac{20}{(1+0.2)^2}(0 + 0.243)\right\} = -1.146$$

$$y_1 = y(1.2) = 0 + \frac{1}{6}[0.4 + 2*0.2 + 2*0.243 + 0.113]$$

$$y_1 = y(1.2) = 0.233$$

Analytical solution

$$y = \frac{1}{2}x^{-2}\sin[4.\ln(x)]$$

$$y(1.2) = 0.23137$$

6.2.3) Runge Kutta – Nystrom Method

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

$$A_j = \frac{1}{2}h.f\left(x_j, y_j, y'_j\right)$$

$$B_j = \frac{1}{2}h.f\left[x_j + \frac{1}{2}h, y_j + \frac{1}{2}h\left(y'_j + \frac{1}{2}A_j\right), y'_j + A_j\right]$$

$$C_j = \frac{1}{2}h.f\left[x_j + \frac{1}{2}h, y_j + \frac{1}{2}h\left(y'_j + \frac{1}{2}A_j\right), y'_j + B_j\right]$$

$$D_j = \frac{1}{2}h.f\left[x_j + h, y_j + h\left(y'_j + C_j\right), y'_j + 2.C_j\right]$$

$$y_{j+1} = y_j + h\left[y'_j + \frac{1}{3}\left(A_j + B_j + C_j\right)\right]$$

$$y'_{j+1} = y'_j + \frac{1}{3}\left[A_j + 2.B_j + 2.C_j + D_j\right]$$

Since it is only for 2nd order differential equation, its usage is limited.

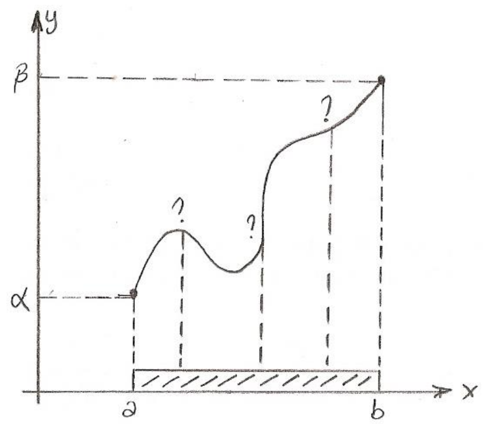
HOMEWORK

1) Differential equation $y'' = x - 4.y^2 + 3.e^{-y'}$ is given with initial conditions of $y(2) = 3$ and $y'(2) = 4$. By choosing $h = 0.1$, calculate $y(5)$.

2) Differential equation $y'' = x^2 - \cos(y) + 2.e^{-x}.y'$ is given with initial conditions of $y(1) = 1$ and $y'(1) = 3$. By choosing $h = 0.1$, calculate $y(5)$.

6.3) Numerical Solution of Second Order Boundary Value Problems

$$y'' = f(x, y, y') \qquad y(a) = \alpha \qquad y(b) = \beta$$



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

$$x_j = x_0 + j.h$$

$$x_j = a + j.h$$

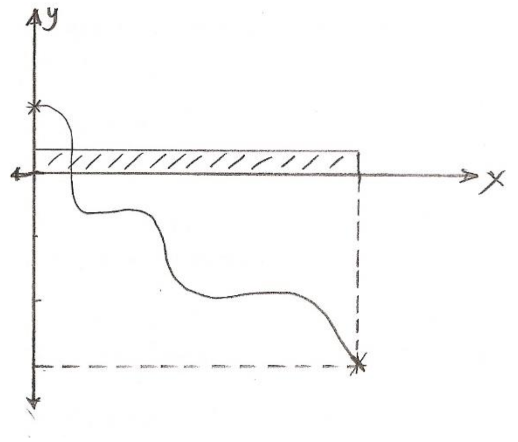
$$y''_j = f(x_j, y_j, y'_j)$$

$$y'_j = \frac{y_{j+1} - y_{j-1}}{2.h} + O(h^2)$$

$$y''_j = \frac{y_{j-1} - 2.y_j + y_{j+1}}{h^2} + O(h^2)$$

If we substitute and rearrange the finite difference formulas in the differential equation, then if $j = 1,2,3,......,n-1$ is chosen, we get (n-1) algebraic equations. If we substitute the boundary conditions $y(a) = \alpha$ and $y(b) = \beta$ properly in this (n-1) equation, we get an (n-1) set of equations. By solving this (n-1) equation, values of y_1, y_2, y_3, ……, y_{n-1} can be found.

Example: Differential equation $y'' = x - 2y + y'$ with boundary conditions $y(0) = 1$ and $y(1) = -3$ is given. If $n = 10$ is chosen, solve the differential equation numerically.



$$h = \frac{b-a}{n} = \frac{1-0}{10} = 0.1$$

$$y''_j = x_j - 2y_j + y'_j$$

If we use the central difference formulas,

=> $$\frac{y_{j-1}-2.y_j+y_{j+1}}{h^2}=x_j-2.y_j+\frac{y_{j+1}-y_{j-1}}{2.h}$$

=> $$\left(1+\frac{h}{2}\right)y_{j-1}+\left(-2+2h^2\right)y_j+\left(1-\frac{h}{2}\right)y_{j+1}=h^2.x_j$$

$x_j = x_0 + j.h$ => $x_j = 0.1 * j$

$$1.05 * y_{j-1} - 1.98 * y_j + 0.95 * y_{j+1} = 0.001 * j$$

Except "j=0" and "j=10", for j=1,2,3…, (n-1) values, the set of linear equations:

$$1.05 * y_0 - 1.98 * y_1 + 0.95 * y_2 = 0.001 \qquad j = 1$$

$$1.05 * y_1 - 1.98 * y_2 + 0.95 * y_3 = 0.002 \qquad j = 2$$

$$1.05 * y_2 - 1.98 * y_3 + 0.95 * y_4 = 0.003 \qquad j = 3$$

$$1.05 * y_3 - 1.98 * y_4 + 0.95 * y_5 = 0.004 \qquad j = 4$$

$$1.05 * y_4 - 1.98 * y_5 + 0.95 * y_6 = 0.005 \qquad j = 5$$

$$1.05 * y_5 - 1.98 * y_6 + 0.95 * y_7 = 0.006 \qquad j = 6$$

$$1.05 * y_6 - 1.98 * y_7 + 0.95 * y_8 = 0.007 \qquad j = 7$$

$$1.05 * y_7 - 1.98 * y_8 + 0.95 * y_9 = 0.008 \qquad j = 8$$

$$1.05 * y_8 - 1.98 * y_9 + 0.95 * y_{10} = 0.009 \qquad j = 9$$

If the boundary conditions are entered, the first and last equations become:

$y(0) = y_0 = 1$

$1.05 * 1 - 1.98 * y_1 + 0.95 * y_2 = 0.001$ => $-1.98 * y_1 + 0.95 * y_2 = -1.049$

$y(1) = y_{10} = -3$

$1.05 * y_8 - 1.98 * y_9 + 0.95 * -3 = 0.009$ => $1.05 * y_8 - 1.98 * y_9 = 2.8590$

Matrix created with equations,

$$\begin{bmatrix} -1.98 & 0.95 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1.05 & -1.98 & 0.95 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1.05 & -1.98 & 0.95 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1.05 & -1.98 & 0.95 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1.05 & -1.98 & 0.95 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1.05 & -1.98 & 0.95 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1.05 & -1.98 & 0.95 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1.05 & -1.98 & 0.95 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1.05 & -1.98 \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \\ y_5 \\ y_6 \\ y_7 \\ y_8 \\ y_9 \end{bmatrix} = \begin{bmatrix} -1.049 \\ 0.002 \\ 0.003 \\ 0.004 \\ 0.005 \\ 0.006 \\ 0.007 \\ 0.008 \\ 2.8590 \end{bmatrix}$$

$y_0 = 1$

$y_1 = 0.7299$ $\quad$ $y_4 = -0.3231$ $\quad$ $y_7 = -1.6371$

$y_2 = 0.4171$ $\quad$ $y_5 = -0.7406$ $\quad$ $y_8 = -2.0991$

$y_3 = 0.0646$ $\quad$ $y_6 = -1.1813$ $\quad$ $y_9 = -2.5571$

$y_{10} = -3$

HOMEWORK

1) Differential equation $y'' = x - 2y + y'$ with boundary conditions $y(0) = 1$ and $y(1) = -3$ is given. By choosing n=100, solve the problem.

2) Differential equation $y'' = x^2 - 4.y + 4.y'$ with boundary conditions $y(1) = -2$ and $y(2) = 4$ is given. By choosing n=100, solve the problem.

6.3.1) Mixed Boundary Condition

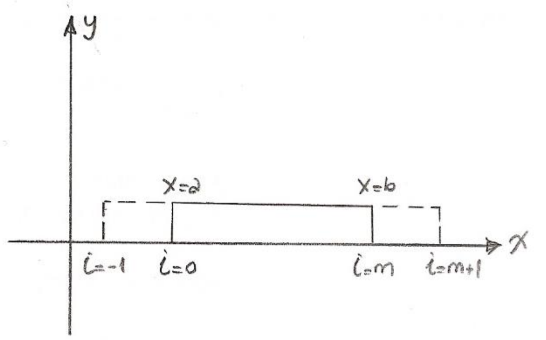
The most general expression of boundary conditions that can be encountered in boundary value problems is $\alpha \frac{dy}{dx} + \beta . y = \gamma$. Here α, β and γ are constants. In these boundary conditions; In the case of $\alpha \neq 0$ and $\beta \neq 0$, the condition that arises with these conditions is called the Mixed Boundary Condition. In the case of $\alpha = 0$ and $\beta \neq 0$, the previous boundary condition is obtained and called the Dirichlet Boundary Condition, in the case of $\alpha \neq 0$ and $\beta = 0$ a2 and b2 the Neuman Boundary Condition is obtained

Let's formulate the following differential equation for mixed boundary conditions at both endpoints,

Differential equation is given $\frac{d^2 y}{dx^2} + C.y = f(x)$

$$\left.\begin{array}{lll} \text{at } x = a & \quad & \alpha_1 \frac{dy}{dx} + \beta_1 . y = \gamma_1 \\ \\ \text{At } x = b & \quad & \alpha_2 \frac{dy}{dx} + \beta_2 . y_2 = \gamma_2 \end{array}\right\} \quad \text{Boundary conditions}$$

Under these boundary conditions, nothing can be said between the function values at $x_0 = a$ and $x = b$. $y(a) = y_0$ and $y(b) = y_m$ are unknown. In this case, the number of unknowns is equal to the number of points obtained by dividing the interval into (m) equal parts, that is (m+1).



If we write the finite difference expression of the differential equation, we get

$$\frac{y_{i-1} - 2.y_i + y_{i+1}}{h^2} + C.y_i = f(x_i)$$

$$y_{i-1} + (C.h^2 - 2).y_i + y_{i+1} = h^2.f(x_i) \qquad (1)$$

if i=0 in equation (1),

$$y_{-1} + (C.h^2 - 2).y_0 + y_1 = h^2.f(x_0) \qquad (2)$$

In this equation, the unknown y_{-1} y-1 is encountered. This unknown represents an imaginary point behind $x = a$ to h, i.e. x = a-h. We can make use of the first boundary condition to eliminate this imaginary point outside the range.

$$\alpha_1 \frac{dy}{dx} + \beta_1.y = \gamma_1$$

$$\alpha_1 \left(\frac{y_1 - y_{-1}}{2h} \right) + \beta_1.y_0 = \gamma_1$$

=> $\quad y_{-1} = y_1 - \frac{2.h}{\alpha_1}(\gamma_1 - \beta_1.y_0)$

If this expression is substituted in equation (2) and summed under common factors, the difference equation for the left endpoint is,

$$\left(h^2.C-2+\frac{2.h.\beta_1}{\alpha_1}\right)y_0+2.y_1=h^2.f(x_0)+\frac{2.h.\gamma_1}{\alpha_1}$$ for $i=0$

Likewise, if $i=m$ is written in equation (1) to obtain the difference equation of the right endpoint,

$$y_{m-1}+(C.h^2-2).y_m+y_{m+1}=h^2.f(x_m) \qquad i=m \qquad (3)$$

In this equation, y_{m+1}, represents an imaginary point $x=b+h$. This imaginary point can be eliminated using the second boundary condition.

$$\alpha_2\left(\frac{y_{m+1}-y_{m-1}}{2h}\right)+\beta_2.y_m=\gamma_2$$

=> $$y_{m+1}=y_{m-1}+\frac{2h}{\alpha_2}(\gamma_2-\beta_2.y_m)$$

If this expression is substituted in equation (3) and summed under common factors, the difference equation for the right end point is,

$$2.y_{m-1}+\left(h^2.C-2-\frac{2.h.\beta_2}{\alpha_2}\right)y_m=h^2.f(x_m)-\frac{2.h.\gamma_2}{\alpha_2} \qquad i=m$$

For midpoints $i=1,2,3,......,m-1$, equation (1) is valid.

$$\left(h^2.C-2+\frac{2.h.\beta_1}{\alpha_1}\right)y_0+2.y_1=h^2.f(x_0)+\frac{2.h.\gamma_1}{\alpha_1} \qquad i=0$$

$$y_0+(C.h^2-2).y_1+y_2=h^2.f(x_1) \qquad i=1$$
$$y_1+(C.h^2-2).y_2+y_3=h^2.f(x_2) \qquad i=2$$

$$y_2+\left(C.h^2-2\right).y_3+y_4=h^2.f\left(x_3\right) \qquad i=3$$

.
.
.

$$y_{m-2}+\left(C.h^2-2\right).y_{m-1}+y_m=h^2.f\left(x_{m-1}\right) \qquad i=m-1$$

$$2.y_{m-1}+\left(h^2.C-2-\frac{2.h.\beta_2}{\alpha_2}\right)y_m=h^2.f\left(x_m\right)-\frac{2.h.\gamma_2}{\alpha_2} \qquad i=m$$

Example: Solve the following differential equation for decreasing h values under the given boundary conditions by means of a computer program and compare with the analytical solution.

Differential Equation ; $\quad x.y''-(x+2).y'+2y=0$

Boundary conditions ; $\quad y'(0)=0 \qquad y'(1)=y(1)+\frac{1}{2}$

Analytical Solution ; $\quad y(x)=e^x-\frac{1}{2}\left(x^2+2x+2\right)$

First, let's divide the interval "0-1" into m equal parts, since both of the boundary conditions are of mixed type, the unknown number is $(m+1)$. A general formula for any point x_i is produced by using central difference formulas instead of derivatives in the differential equation.

$$x_i\left[\frac{y_{i-1}-2.y_i+y_{i+1}}{h^2}\right]-\left(x_i+2\right)\left[\frac{y_{i+1}-y_{i-1}}{2.h}\right]+2.y_i=0$$

$$\left[h+\left(1+\frac{h}{2}\right).x_i\right]y_{i-1}+2.\left(h^2-x_i\right).y_i+\left[-h+\left(1-\frac{h}{2}\right).x_i\right]y_{i+1}=0$$

$$x_i = x_0 + i.h$$
$$x_i = i.h$$

If $x_i = i.h$ is substituted divide side by side h,

$$\left[1+\left(1+\frac{h}{2}\right).i\right]y_{i-1} + 2.(h-i).y_i + \left[-1+\left(1-\frac{h}{2}\right).i\right]y_{i+1} = 0 \qquad , \ i = 0,1,2,......,m \qquad (1)$$

If we put $i = 0$ in equation (1), we get,

$$y_{-1} + 2.h.y_0 - y_1 = 0 \qquad i = 0$$

If the left boundary condition is used,

$$y'(0) = 0 \quad => \quad \frac{y_1 - y_{-1}}{2.h} = 0 \quad => \quad y_{-1} = y_1$$

$$=> \quad y_1 + 2.h.y_0 - y_1 = 0$$
$$y_0 = 0 \qquad i = 0$$

If we put $i = m$ in equation (1),

$$\left[1+\left(1+\frac{h}{2}\right).m\right]y_{m-1} + 2.(h-m).y_m + \left[-1+\left(1-\frac{h}{2}\right).m\right]y_{m+1} = 0 \qquad i = m$$

From the second boundary condition,

$$\frac{y_{m+1} - y_{m-1}}{2.h} = y_m + \frac{1}{2}$$

=> $\quad y_{m+1} = y_{m-1} + 2.h.y_m + h$

If this expression is replaced and arranged above;

$$2m.y_{m-1} + \left(2h - h^2 - 2\right)m.y_m = -h\left[-1 + \left(1 - \frac{h}{2}\right)m\right] \qquad \text{for } i = m$$

For $i = 1,2,......,m-1$, from the equation (1), $(m-1)$ equations are also obtained. Thus, the solution is completed by solving m equations with m unknown Gauss method.

x	Numerical Solution				Analytical Solution
	$h = 0.1$ n=10	$h = 0.05$ n=20	$h = 0.0025$ n=400	$h = 0.001$ n=1000	
0.2	0.000935	0.001285	0.001375	0.001398	0.001402
0.4	0.010563	0.011508	0.011745	0.011813	0.011824
0.6	0.039696	0.041510	0.041960	0.042098	0.042110
0.8	0.101570	0.104547	0.105290	0.105508	0.105541
1.0	0.212410	0.216810	0.217915	0.218230	0.218280

6.3.2) The Boundary Condition Given at Infinite

Some differential equations may have a limit value at infinity. If we give an example of this,

Differential equation ; $y'' + C.y = f(x)$

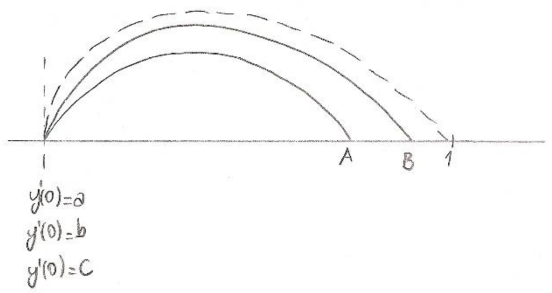
Boundary conditions ; $y(0) = 0$, $y(\infty) = \beta$

In order to solve this problem by creating difference equations, we need to know what order the value specified as infinity is. Since we cannot form an idea about the order of x, we need to solve the problem as an initial value problem. But there is another problem here as well. The one of the initial condition, I mean (y') is missing. In other words, in order to solve the above differential equation, not only $y(0)$, we need to know $y'(0)$ initial value as well as . However, $y'(0)$ value is unknown. By the way, we solve the problem as an initial value problem by making an estimation for the initial condition $y'(0)$ and see where $y'(0)$ is going on the way to $x \to \infty$. In other words, when $y'(0) = a$ is taken, it converges to a value such as $y \to A$ when it goes to $x \to \infty$. Then let's make a second guess for the initial condition; When $y'(0) = b$ is taken, it converges to a value such as $y \to B$ when it goes to $x \to \infty$. Then a new predict value is calculated for $y(\infty) = \beta$ when it goes to infinity . This is a kind of Newton-Rapson application,

$$c = a - \frac{A - \beta}{(A - B)/(a - b)}$$

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

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



This method, which is applied, is called the shooting method.

Example: Solve the following differential equation,

Differential equation ; $y'' - 4.y = 1$

Boundary conditions ; $y(0) = 0$, $y(\infty) = -\dfrac{1}{4}$

To solve the problem as an initial value problem, we reduce the differential equation to a first-order system of equations,

$$y' = p = f_1(x, y, p)$$
$$p' = 1 + 4.y = f_2(x, y, p)$$

$$y(0) = 0$$

If $y'(0) = p(0) = a = 1$ is chosen

If the solution is made,

$$y(\infty) = y(5) = A = 8242$$

If $y'(0) = p(0) = b = -1$ is chosen,

If the solution is made,

$$y(\infty) = y(5) = B = -2749$$

If we put these values into the expression given for "c" above, we get a new predict for the derivative,

$$c = 1 - \frac{8242 - (-1/4)}{(8242 - (-2749))/(1 - (-1))} = -0.499818$$

If we repeat the solution with this new value,

It is found at $y(4.6)=y(\infty)=-0.25$, we see that the solution is fixed. In reality the value of "c" is 0.5. Some equations can be solved several times with the number of predictions Newton-Rapson.

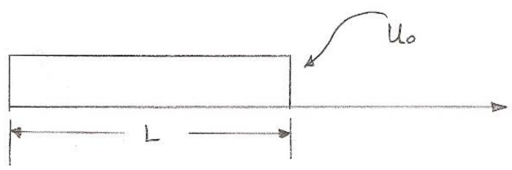
The second boundary condition is not necessarily like $y(\infty)=K$. The shooting method can be applied similarly to boundary value problems such as $y(L)=K$.

7. NUMERICAL SOLUTION OF PARABOLIC EQUATIONS

7.1. Transform into Dimensionless Form

Numerical solutions of problems involve quite a lot of arithmetic operations. Therefore, it is desirable that a solution be valid for as many problems as possible. This solution can be achieved by bringing the desired equation into dimensionless form. For example, although the swing of a pendulum in a viscous medium and the discharge of voltage across a capacitor through resistance and inductance are physically separate, the differential equation governing these two different expressions is exactly the same.

$$\frac{\partial U}{\partial T} = K \frac{\partial^2 U}{\partial X^2}$$



$x = \frac{X}{L}$ (The size of the object has been made dimensionless)

=> $X = x.L$

$u = \frac{U}{U_0}$ => $U = u.U_0$

=> $\frac{\partial u.U_0}{\partial T} = K \frac{\partial^2 u.U_0}{\partial (x.L)^2}$ => $U_0 \frac{\partial u}{\partial T} = KU_0 \frac{\partial^2 u}{L^2.\partial x^2}$

=> $\frac{L^2}{K} \frac{\partial u}{\partial T} = \frac{\partial^2 u}{\partial x^2}$,if $t = \frac{K.T}{L^2}$, $T = \frac{L^2}{K} t$ becomes

$$\frac{L^2}{K}\frac{\partial u}{\partial\left(\frac{L^2}{K}t\right)}=\frac{\partial^2 u}{\partial x^2} \qquad => \qquad \frac{\partial u}{\partial t}=\frac{\partial^2 u}{\partial x^2}$$

7.2. Explicit Solution Method

The one-dimensional, time-dependent conduction heat equation is a parabolic equation and its formula is as follows,

$$\frac{\partial u}{\partial t}=\frac{\partial^2 u}{\partial x^2}$$

$u(x,t)=u_{i,j}$ $\qquad i=x$ and $j=t$

The first-degree derivative expression on the left side of the equation must be opened with the forward difference formula (Due to stability and convergence problem). Although the right side of the equation is usually opened with the central difference formula, it can also be opened with the forward and backward difference formulas, if desired.

$$\frac{u_{i,j+1}-u_{i,j}}{\delta t}=\frac{u_{i-1,j}-2.u_{i,j}+u_{i+1,j}}{(\delta x)^2}$$, FTCS (Forward Time Central Space)

$$u_{i,j+1}=r.u_{i-1,j}+(1-2.r)u_{i,j}+r.u_{i+1,j} \qquad \text{and} \qquad r=\frac{\delta t}{(\delta x)^2}$$

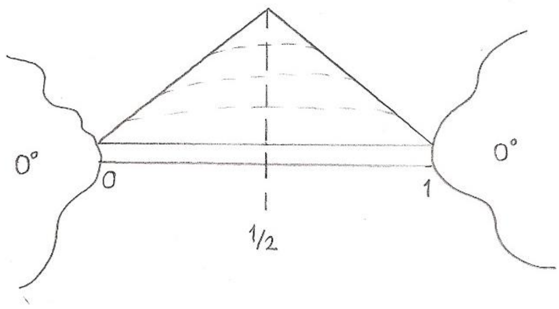
$u_{i,j+1}$, $(i, j+1)$ is the unknown temperature at the lattice point. If the temperatures in the j step are known, the temperatures in the $j+1$ time step can be calculated with the finite difference formula above. Since the temperatures at the first moment, that is, at the moment $j=0$, are given, the temperatures in the step $j=1,2,3,......,n$ are calculated step by step. This method is called the explicit solution method.

Example: The initial temperature of the stick (in dimensionless form) whose ends are in contact with a melting ice block is given by

$$u(x,0) = 2.x \qquad 0 \le x \le \frac{1}{2}$$

$$u(x,0) = 2.(1-x) \qquad \frac{1}{2} \le x \le 1$$

Calculate the change in temperature of the rod with time.



$$\left.\begin{array}{ll} u(x,0) = 2.x & 0 \le x \le \frac{1}{2} \\ & \\ u(x,0) = 2.(1-x) & \frac{1}{2} \le x \le 1 \end{array}\right\} \quad \text{Initial condition}$$

$$\left.\begin{array}{l} u(0,t) = 0 \\ \\ u(1,t) = 0 \end{array}\right\} \quad \text{Boundary conditions}$$

Finite difference expression,

$$u_{i,j+1} = r.u_{i-1,j} + (1-2.r)u_{i,j} + r.u_{i+1,j} \qquad \text{and} \qquad r = \frac{\delta t}{(\delta x)^2}$$

Since the system is symmetrical, it will be sufficient to solve half of it.

Case 1: Let's take $n = 10$ (divide the bar into 10 parts)

Let’s choose $\delta x = \frac{1}{10} = 0.1$ and $\delta t = \frac{1}{1000}$

$$r = \frac{\delta t}{(\delta x)^2} = 0.1$$

=> $u_{i,j+1} = 0.1 * u_{i-1,j} + 0.8 * u_{i,j} + 0.1 * u_{i+1,j}$

$$u_{i,j+1} = \frac{1}{10}\left(u_{i-1,j} + 8.u_{i,j} + u_{i+1,j}\right)$$

$x_i = x_0 + i.\delta x$ => $x_i = 0.1 * i$

	$i=0$ $x=0$	$i=1$ $x=0.1$	$i=2$ $x=0.2$	$i=3$ $x=0.3$	$i=4$ $x=0.4$	$i=5$ $x=0.5$	. . . . .	$i=10$ $x=1$
$t=0.000$	0	0.2	0.4	0.6	0.8	1	. . . . .	.
$t=0.001$	0	0.2	0.4	0.6	0.8	0.96	. . . . .	.
$t=0.002$	0	0.2	0.4	0.6	0.7960	0.9280	. . . . .	.
$t=0.003$	0	0.2	0.4	0.5996	0.7816	0.9016	. . . . .	.
.	.	.	.	.	.	.	.	.
.	.	.	.	.	.	.	.	.
.	.	.	.	.	.	.	.	.
$t=0.01$	0	0.1996	0.3968	0.5822	0.7281	0.7867	. . . . .	
.	.	.	.	.	.	.	.	.
.	.	.	.	.	.	.	.	.
.	.	.	.	.	.	.	.	.
$t=0.02$	0	0.1938	0.3781	0.5373	0.6486	0.6891	. . . . .	.

If $x_i = 0.1 * i$,

$u(x,0) = 2.x$ $\quad 0 \le x \le \frac{1}{2}$ => $u_{i,0} = 2.x = 0.2 * i$ $\quad 0 \le x \le \frac{1}{2}$

$u(x,0) = 2.(1-x) \qquad \frac{1}{2} \le x \le 1 \qquad => \qquad u(x,0) = 2.(1-x) = 2.(1-0.1*i) \qquad \frac{1}{2} \le x \le 1$

Analytical solution of differential equation,

$$u = \frac{8}{\pi^2}\sum_{n=1}^{\infty}\frac{1}{n^2}\left(\sin\frac{1}{2}n.\pi\right)(\sin n.\pi.x).e^{-n^2\pi^2 t}$$

	Finite Difference Solution at $x = 0.3$	Analytical Solution at $x = 0.3$	Difference	Percentage Error
$t = 0.01$	0.5822	0.5799	0.0023	0.4
$t = 0.02$	0.5373	0.5334	0.0039	0.7
$t = 0.1$	0.2472	0.2444	0.0028	1.1

Case 2: Let's take $n = 10$ (divide the bar into 10 parts)

Let's choose $\delta x = \frac{1}{10} = 0.1$ and $\delta t = \frac{5}{1000} = 0.005$

$$r = \frac{\delta t}{(\delta x)^2} = 0.5$$

=> $u_{i,j+1} = 0.5 * u_{i-1,j} + 0.5 * u_{i+1,j} = \frac{1}{2}\left(u_{i-1,j} + u_{i+1,j}\right)$

	$i = 0$ $x = 0$	$i = 1$ $x = 0.1$	$i = 2$ $x = 0.2$	$i = 3$ $x = 0.3$	$i = 4$ $x = 0.4$	$i = 5$ $x = 0.5$	. . . . .	$i = 10$ $x = 1$
$t = 0.000$	0	0.2	0.4	0.6	0.8	1	. . . . .	.
$t = 0.005$	0	0.2	0.4	0.6	0.8	0.8	. . . . .	.
$t = 0.01$	0	0.2	0.4	0.6	0.7	0.8	. . . . .	.
$t = 0.015$	0	0.2	0.4	0.55	0.7	0.7	. . . . .	.
.	.	.	.	.	.	.	.	.
.	.	.	.	.	.	.	.	.

.	.	.	.	.	.	.	.	.
$t=0.1$	0	0.0949	0.1717	0.2484	0.2778	0.3071	. . . . .	.

	Finite Difference Solution at $x=0.3$	Analytical Solution at $x=0.3$	Difference	Percentage Error
$t=0.005$	0.6	0.5966	0.0034	0.57
$t=0.01$	0.6	0.5799	0.0201	3.5
$t=0.02$	0.55	0.5334	0.0166	3.1
$t=0.1$	0.2484	0.2444	0.0040	1.6

Case 3: Let's take $n=10$ (divide the bar into 10 parts)

Let's choose $\delta x=\frac{1}{10}=0.1$ and $\delta t=\frac{1}{100}=0.01$

$$r=\frac{\delta t}{(\delta x)^2}=1$$

=> $u_{i,j+1}=u_{i-1,j}-u_{i,j}+u_{i+1,j}$

	$i=0$ $x=0$	$i=1$ $x=0.1$	$i=2$ $x=0.2$	$i=3$ $x=0.3$	$i=4$ $x=0.4$	$i=5$ $x=0.5$	. . . . .	$i=10$ $x=1$
$t=0.000$	0	0.2	0.4	0.6	0.8	1.0	. . . . .	.
$t=0.01$	0	0.2	0.4	0.6	0.8	0.6	. . . . .	.
$t=0.02$	0	0.2	0.4	0.6	0.4	1.0	. . . . .	.
$t=0.03$	0	0.2	0.4	0.2	1.2	-0.2		
$t=0.04$	0	0.2	0.4	1.4	-1.2	2.6	. . . . .	.
.	.	.	.	.	.	.	.	.
.	.	.	.	.	.	.	.	.
.	.	.	.	.	.	.	.	.

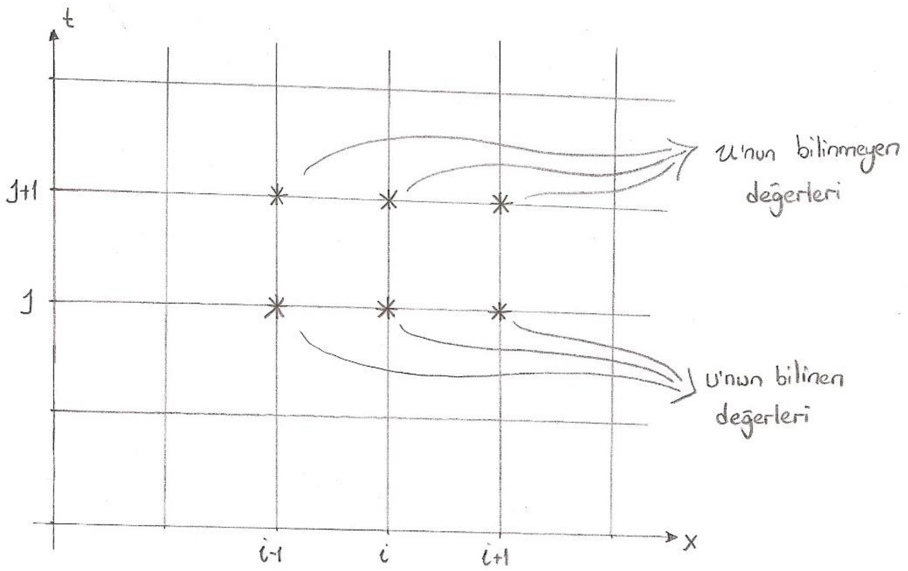
The solution is completely pointless. These 3 case studies show that the r value is an important parameter. In the explicit method, the solution range is valid for $0 \le r \le \frac{1}{2}$. Later, this limitation will be analytically demonstrated on stability and convergence issues.

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \quad \Rightarrow \quad r_1 = \frac{\delta t}{(\delta x)^2},\; r_2 = \frac{\delta t}{(\delta y)^2} \text{ and it must be } r_1, r_2 \le \frac{1}{4}$$

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} \quad \Rightarrow \quad r_1 = \frac{\delta t}{(\delta x)^2},\; r_2 = \frac{\delta t}{(\delta y)^2},\; r_2 = \frac{\delta t}{(\delta z)^2} \text{ and } r_1, r_2, r_3 \le \frac{1}{8}$$

7.3. Crank-Nicolson Implicit Method

Although the Explicit method is computationally simple, it has a very important shortcoming. The time digit δt must be taken very, very small. Because the calculations are valid for the $0 \le r \le \frac{1}{2}$ range. Therefore, δt should be taken very small in order to obtain sufficiently accurate results. If the δt value is taken too small, the computational load increases. In 1947, Crank-Nicolson proposed a method that reduces the computational volume and is valid for all values. They thought that the partial differential equation was valid at the midpoints of the lattice points and took the finite differences of $\frac{\partial^2 u}{\partial x^2}$ as the mean of the approximations at the lattice points j and $j+1$.



$$\frac{\partial u}{\partial t}=\frac{\partial^2 u}{\partial x^2}$$

$$\frac{u_{i,j+1}-u_{i,j}}{\delta t}=\frac{1}{2}\frac{u_{i-1,j}-2*u_{i,j}+u_{i+1,j}}{(\delta x)^2}+\frac{1}{2}\frac{u_{i-1,j+1}-2*u_{i,j+1}+u_{i+1,j+1}}{(\delta x)^2}$$

$$\frac{u_{i,j+1}-u_{i,j}}{\delta t}=\beta\frac{u_{i-1,j}-2*u_{i,j}+u_{i+1,j}}{(\delta x)^2}+(1-\beta)\frac{u_{i-1,j+1}-2*u_{i,j+1}+u_{i+1,j+1}}{(\delta x)^2}$$

$\beta=1$: Explicit method

$\beta=\frac{1}{2}$: Crank-Nicolson Implicit Method

$\beta=0$: Full Implicit Method

If $\beta=\frac{1}{2}$ is chosen,

$$-r.u_{i-1,j+1}+(2+2.r).u_{i,j+1}-r.u_{i+1,j+1}=r.u_{i-1,j}+(2-2.r).u_{i,j}+r.u_{i+1,j}$$

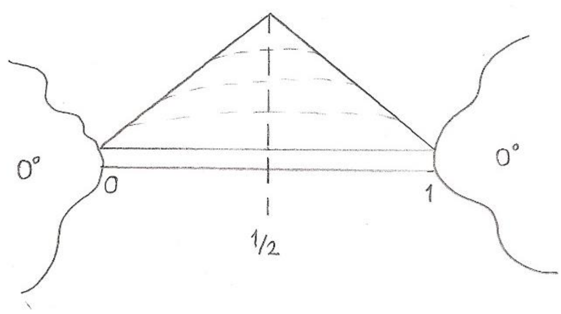
There are 3 unknown $j+1$ terms on the left side of the finite difference expression and 3 known (j) expressions on the right side. If there are $(n-1)$ inner lattice points during each time step (For example, $j=0$ and $i=1,2,......,n-1$) $(n-1)$ sets of interconnected equations are obtained and $(n-1)$ will be unknown. Since the u values are given as the first condition and the boundary conditions are given during the time at the first time $(j=0)$, the u values at the $j=1$ order are found from the data at the $j=0$ time order. This method is defined as the Implicit method.

Example: Solve the previous example using the Crank-Nicolson method.

$$\frac{\partial u}{\partial t}=\frac{\partial^2 u}{\partial x^2}$$

$$\left.\begin{aligned} u(x,0)&=2.x && 0\le x\le \frac{1}{2} \\ u(x,0)&=2.(1-x) && \frac{1}{2}\le x\le 1 \end{aligned}\right\} \quad \text{Initial condition}$$

$$\left.\begin{aligned} u(0,t)&=0 \\ u(1,t)&=0 \end{aligned}\right\} \quad \text{Boundary conditions}$$



If $n = 10$ i.e. $\delta x = \frac{1}{10} = 0.1$ and if we choose $\delta t = \frac{1}{100} = 0.01$

=> $r = \frac{\delta t}{(\delta x)^2} = 1$

=> $-u_{i-1,j+1} + 4.u_{i,j+1} - u_{i+1,j+1} = u_{i-1,j} + u_{i+1,j}$

If we take $j = 0$, $i = 1,2,3,......,n-1(9)$ (It is sufficient to calculate up to $i = 5$ since it is symmetrical)

If we take $j = 0$,

$-u_{0,1} + 4.u_{1,1} - u_{2,1} = u_{0,0} + u_{2,0}$ $\quad i = 1$

$-u_{1,1} + 4.u_{2,1} - u_{3,1} = u_{1,0} + u_{3,0}$ $\quad i = 2$

$-u_{2,1} + 4.u_{3,1} - u_{4,1} = u_{2,0} + u_{4,0}$ $\quad i = 3$

$-u_{3,1} + 4.u_{4,1} - u_{5,1} = u_{3,0} + u_{5,0}$ $\quad i = 4$

$-u_{4,1} + 4.u_{5,1} - u_{6,1} = u_{4,0} + u_{6,0}$ $\quad i = 5$

Since $x_i = 0.1 * i$,

$u(x,0) = 2.x \quad 0 \le x \le \frac{1}{2}$ => $u_{i,0} = 2.x = 0.2 * i \quad 0 \le x \le \frac{1}{2}$

$u(x,0) = 2.(1-x) \quad \frac{1}{2} \le x \le 1$ => $u(x,0) = 2.(1-x) = 2.(1-0.1*i) \quad \frac{1}{2} \le x \le 1$

$-u_{0,1} + 4.u_{1,1} - u_{2,1} = 0.0 + 0.4$ $\quad i = 1$ $\quad$ ($u_{0,1} = 0$)

$-u_{1,1} + 4.u_{2,1} - u_{3,1} = 0.2 + 0.6$ $\quad i = 2$

$-u_{2,1} + 4.u_{3,1} - u_{4,1} = 0.4 + 0.8$ $\quad i = 3$

$-u_{3,1} + 4.u_{4,1} - u_{5,1} = 0.6 + 1.0$ $\quad i = 4$

$$-u_{4,1}+4.u_{5,1}-u_{6,1}=0.8+0.8 \qquad i=5 \qquad (u_{4,0}=u_{6,0} \text{ and } u_{4,1}=u_{6,1})$$

Unknowns *Knowns*

$$-u_0+4.u_1-u_2=u_0+u_2 \qquad i=1 \qquad (u_{0,1}=0)$$

$$-u_1+4.u_2-u_3=u_1+u_3 \qquad i=2$$

$$-u_2+4.u_3-u_4=u_2+u_4 \qquad i=3$$

$$-u_3+4.u_4-u_5=u_3+u_5 \qquad i=4$$

$$-u_4+4.u_5-u_6=u_4+u_6 \qquad i=5 \qquad (u_{4,0}=u_{6,0} \text{ and } u_{4,1}=u_{6,1})$$

$$\begin{array}{c} \begin{array}{ccccc} u_1 & u_2 & u_3 & u_4 & u_5 \end{array} \\ \begin{bmatrix} 4 & -1 & 0 & 0 & 0 \\ -1 & 4 & -1 & 0 & 0 \\ 0 & -1 & 4 & -1 & 0 \\ 0 & 0 & -1 & 4 & -1 \\ 0 & 0 & 0 & -2 & 4 \end{bmatrix} \end{array} \begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \\ u_5 \end{bmatrix} = \begin{bmatrix} 0.0+0.4 \\ 0.2+0.6 \\ 0.4+0.8 \\ 0.6+1.0 \\ 0.8+0.8 \end{bmatrix}$$

$u_1=0.1989$ $\qquad$ $u_2=0.3956$

$u_3=0.5834$ $\qquad$ $u_4=0.7381$

$u_5=0.7691$

If $j=1$,

$$-u_0+4.u_1-u_2=u_0+u_2=0+0.3956 \qquad i=1 \qquad (u_{0,1}=0)$$

$$-u_1+4.u_2-u_3=u_1+u_3=0.1989+0.5834 \qquad i=2$$

$$-u_2+4.u_3-u_4=u_2+u_4=0.3956+0.7381 \qquad i=3$$

$$-u_3+4.u_4-u_5=u_3+u_5=0.5834+0.7691 \qquad i=4$$

$$-u_4+4.u_5-u_6=u_4+u_6=0.7381+0.7381 \qquad i=5 \qquad (u_{4,0}=u_{6,0} \text{ and } u_{4,1}=u_{6,1})$$

	$i=0$ $x=0$	$i=1$ $x=0.1$	$i=2$ $x=0.2$	$i=3$ $x=0.3$	$i=4$ $x=0.4$	$i=5$ $x=0.5$	. . . . .	$i=10$ $x=1$
$t=0.000$	0	0.2	0.4	0.6	0.8	1.0	. . . . .	.
$t=0.01$	0	0.1989	0.3956	0.5834	0.7381	0.7691	. . . . .	.
$t=0.02$	0	0.1936	0.3789	0.5400	0.6461	0.6921	. . . . .	.
. . .	0	. . .	. . .	. . .	. . .	. . .	. . .	. . .
$t=0.1$	0	0.0948	0.1803	0.2482	0.2918	0.3069	. . . . .	.
$t=0.1$ (Analytical Solution)	0	0.0934	0.1776	0.2444	0.2873	0.3021	. . . . .	.

The Crank-Nicolson method is stable for all r values. But for large values of r (around 40), undesirable finite oscillations occur in numerical solutions. The problem can be solved systematically with the method of Gauss and Gauss-Jordan elimination.

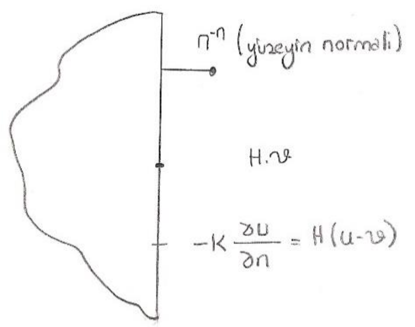
HOMEWORK:

1) Solve the question in the previous Example with the fully implicit (closed) method.

7.4. Derivative Type Boundary Conditions

In practice, derivative-type boundary conditions are frequently encountered. For example, if a surface is thermally isolated, that is, there is no heat transfer perpendicular to this surface, the boundary condition is $\frac{\partial u}{\partial n}=0$ everywhere on this surface. Similarly, if a surface with temperature u is in contact with a fluid with temperature v, the condition that the heat transfer by conduction equals the heat transfer by convection can be given as $-K\frac{\partial u}{\partial n} = H.(u - v)$.

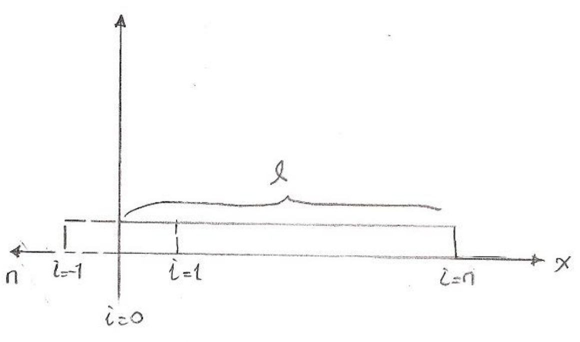
Here, K is the heat transfer coefficient (thermal conductivity) of the material and H (film coefficient) is the heat transfer coefficient of the surface.



$$\frac{\partial u}{\partial n} = -h.(u - v)$$

$h = \frac{H}{K}$ (positive coefficient)

Let the surface of a rod of length L be thermally insulated and allow the heat to be transferred by convection at $x = 0$. At time t, the temperature at this end will be unknown. It can be determined this by using the boundary condition.



$$-\frac{\partial u}{\partial x} = -h.(u - v)$$

Since $x = 0$ is the left end and in the opposite direction to the normal x-axis outward from the boundary condition, the $(-)$ sign is placed at the beginning of the expression.

$$\frac{\partial u}{\partial x} = h.(u - v)\Big|_{x=0}$$

If we write the forward difference finite difference expression,

$$\frac{u_{1,j} - u_{0,j}}{\delta x} = h\left(u_{0,j} - v\right)$$

Thus we get an additional equation for $u_{0,j}$.

If we want to express $\frac{\partial u}{\partial n}$ more precisely, we can open the first derivative with the central difference formula,

$$\frac{u_{1,j} - u_{-1,j}}{2.\delta x} = h\left(u_{0,j} - v\right)$$

$u_{-1,j}$ is an imaginary temperature and is the temperature of the outer lattice point outside the domain $(-\delta x, j\delta t)$. $u_{-1,j}$ is an unknown temperature and another equation is needed for the solution. This can be achieved by obtaining one more equation, assuming that the finite difference expression of the differential equation is also satisfied at the point $x = 0$ of the bar. Similar equations can be used for the point of the bar at $x = l$.

Example: Solve the equation $\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}$ with the explicit method for the following boundary and initial conditions. Use the central difference expression for the boundary conditions.

$u(x,0) = 1$ => Initial condition

$$\left.\begin{aligned} \frac{\partial u(0,t)}{\partial x} &= u(0,t) \\ \frac{\partial u(1,t)}{\partial x} &= -u(1,t) \end{aligned}\right\} \quad \text{Boundary conditions}$$

$$\frac{u_{i,j+1} - u_{i,j}}{\delta t} = \frac{u_{i-1,j} - 2 * u_{i,j} + u_{i+1,j}}{(\delta x)^2}$$

=> $u_{i,j+1} = u_{i,j} + r\left(u_{i-1,j} - 2.u_{i,j} + u_{i+1,j}\right)$ and $r = \frac{\delta t}{(\delta x)^2}$

$i = 0,1,2,......,n-1,n$ Since the derivative type is the boundary condition and central differences are used in this equation, it is valid for the values of "0" and "n ".

$$u_{0,j+1} = u_{0,j} + r\left(u_{-1,j} - 2.u_{0,j} + u_{1,j}\right)$$

$\frac{\partial u(0,t)}{\partial x} = u(0,t)$ => $\frac{u_{1,j} - u_{-1,j}}{2.\delta x} = u_{0,j}$

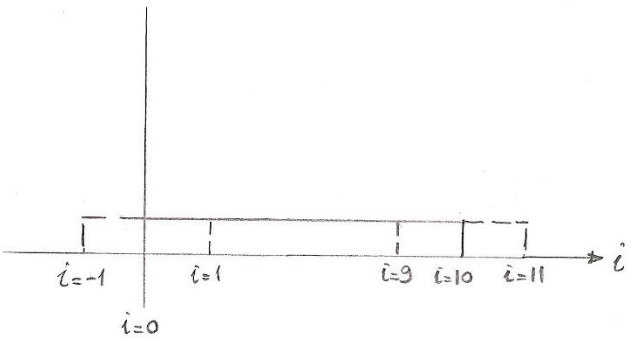
=> $u_{-1,j} = u_{1,j} - 2.\delta x.u_{o,j}$

From the general equation $u_{0,j+1} = u_{0,j} + r\left(u_{1,j} - 2.\delta x.u_{o,j} - 2.u_{0,j} + u_{1,j}\right)$,

$$u_{0,j+1} = u_{0,j} + 2r\left(u_{1,j} - (1+\delta x)u_{0,j}\right) \qquad \text{for } i = 0$$

If $n = 10$ is chosen,

$$n = 10 \qquad => \qquad \delta x = \frac{1}{10} = 0.1$$



If $i = 10$,

$$u_{10,j+1} = u_{10,j} + r\left(u_{9,j} - 2.u_{10,j} + u_{11,j}\right)$$

$$\frac{u_{11,j} - u_{9,j}}{2.\delta x} = -u_{10,j} \qquad => \qquad u_{11,j} = u_{9,j} - 2.\delta x.u_{10,j}$$

$$u_{10,j+1} = u_{10,j} + r\left(u_{9,j} - 2.u_{10,j} + u_{9,j} - 2.\delta x.u_{10,j}\right)$$

$$u_{10,j+1} = u_{10,j} + 2r.\left(u_{9,j} - (1+\delta x)u_{10,j}\right) \qquad \text{for } i = n = 10,$$

The first and last boundary conditions show that the equations are symmetrical. In this case, it is sufficient to take half of the system and make a solution.

The solution is valid for $r \le \dfrac{1}{2+\delta x}$.

If $r = \dfrac{1}{4}$ is chosen, $r = \dfrac{\delta t}{(\delta x)^2}$ => $\delta t = r.(\delta x)^2 = 0.0025$

$$u_{0,j+1} = u_{0,j} + \frac{1}{2}\left[u_{1,j} - 1.1 * u_{0,j}\right]$$

$$u_{0,j+1} = \frac{1}{2}\left[0.9 * u_{0,j} + u_{1,j}\right] \qquad i = 0$$

$$u_{i,j+1} = \frac{1}{4}\left[u_{i-1,j} + 2 * u_{i,j} + u_{i+1,j}\right] \qquad i = 1,2,3,4,5$$

$$x_i = x_0 + i * \delta x \qquad => \qquad x_i = 0.1 * i$$

	$i=0$ $x=0$	$i=1$ $x=0.1$	$i=2$ $x=0.2$	$i=3$ $x=0.3$	$i=4$ $x=0.4$	$i=5$ $x=0.5$
$t=0.000$	1.0	1.0	1.0	1.0	1.0	1.0
$t=0.0025$	0.95	1.0	1.0	1.0	1.0	1.0
$t=0.0050$	0.9275	0.9875	1.0	1.0	1.0	1.0
.	.	.	.	.	.	.
$t=0.100$	0.7175	0.7829	0.8345	0.8718	0.8942	0.9017
$t=0.250$	0.5542	0.6048	0.6492	0.6745	0.6923	0.6983
$t=0.500$	0.3612	0.3942	0.4205	0.4396	0.4512	0.4551
$t=1.000$	0.1534	0.1674	0.1786	0.1867	0.1917	0.1933

The analytical solution of this differential equation is

$$u = 4\sum_{n=1}^{\infty}\left\{\frac{\sec(\alpha_n)}{(3+4.\alpha_n^2)}e^{-4.\alpha_n^2.t}Cos2\alpha_n(x-\frac{1}{2})\right\} \qquad (0<x<1)$$

Here α_n is the positive roots of the $\alpha.\tan\alpha = \frac{1}{2}$ function.

	$i=0$ $x=0$	$i=1$ $x=0.1$	$i=2$ $x=0.2$	$i=3$ $x=0.3$	$i=4$ $x=0.4$	$i=5$ $x=0.5$
$t=0.000$	1.0	1.0	1.0	1.0	1.0	1.0
$t=0.0025$	0.9400	0.9951	0.9999	1.0	1.0	1.0
$t=0.0050$	0.9250	0.9841	0.9984	0.9999	1.0	1.0
.	.	.	.	.	.	.
$t=0.100$	0.7176	0.7828	0.8342	0.8713	0.8936	0.9010
$t=0.250$	0.5546	0.6052	0.6454	0.6747	0.6924	0.6984
$t=0.500$	0.3619	0.3949	0.4212	0.4403	0.4519	0.4558
$t=1.000$	0.1542	0.1682	0.1794	0.1875	0.1925	0.1941

Example: Solve the same problem with the forward (backward) finite difference expansion for boundary conditions and the differential equation with the explicit method.

$$\frac{\partial u}{\partial t}=\frac{\partial^2 u}{\partial x^2} \qquad => \qquad \frac{u_{i,j+1}-u_{i,j}}{\delta t}=\frac{u_{i-1,j}-2.u_{i,j}+u_{i+1,j}}{(\delta x)^2}$$

=> $u_{i,j+1}=u_{i,j}+r.(u_{i-1,j}-2.u_{i,j}+u_{i+1,j})$ and $r=\frac{\delta t}{(\delta x)^2}$

In this case, it is valid for $i=1,2,3,......,n-1$ (forward and backward difference expansion applied to the boundary conditions)

If $i=1$,

$$u_{1,j+1}=u_{1,j}+r.(u_{0,j}-2.u_{1,j}+u_{2,j}) \qquad i=1$$

If we write the forward difference expression of the boundary condition at $x=0$,

$$\frac{\partial u(0,t)}{\delta x}=u(0,t) \qquad => \qquad \frac{u_{1,j}-u_{0,j}}{\delta x}=u_{0,j}$$

$$=> \qquad u_{0,j}=\frac{u_{1,j}}{1+\delta x} \qquad u_{0,j+1}=\frac{u_{1,j+1}}{1+\delta x}$$

$$u_{1,j+1}=u_{1,j}+r.\left(\frac{u_{1,j}}{1+\delta x}-2.u_{1,j}+u_{2,j}\right)$$

$$u_{1,j+1}=\left(1-2r+\frac{r}{1+\delta x}\right)u_{1,j}+r.u_{2,j}$$ for $i=1$,

If $\delta x=0.1$ and $r=\frac{1}{4}$ is chosen,

$\delta t=0.0025$ becomes,

$$u_{1,j+1}=\frac{8}{11}u_{1,j}+\frac{1}{4}u_{2,j} \qquad i=1$$

$$u_{0,j+1}=\frac{u_{1,j+1}}{1.1}$$

$$u_{i,j+1}=\frac{1}{4}\left(u_{i-1,j}+2.u_{i,j}+u_{i+1,j}\right) \qquad i=2,3,4,5$$

For $x = 0.1 * i$,

	$i=0$ $x=0$	$i=1$ $x=0.1$	$i=2$ $x=0.2$	$i=3$ $x=0.3$	$i=4$ $x=0.4$	$i=5$ $x=0.5$
$t=0.000$	1.0	1.0	1.0	1.0	1.0	1.0
$t=0.0025$	0.8884	<= 0.9773	1.0	1.0	1.0	1.0
$t=0.0050$	0.8734	<= 0.9607	0.9943	1.0	1.0	1.0
.	.	.	.	.	.	.
.	.	.	.	.	.	.
.	.	.	.	.	.	.
$t=0.100$	0.6869	<= 0.7556	0.8102	0.8498	0.8738	0.8818
$t=0.250$	0.5206	<= 0.5727	0.6142	0.6444	0.6628	0.6689
$t=0.500$	0.3283	<= 0.3611	0.3873	0.4063	0.4179	0.4218
$t=1.000$	0.1305	<= 0.1435	0.1540	0.1615	0.1661	0.1677

HOMEWORK

1) Solve the same problem with the Crank-Nicolson method. For derivative boundary conditions, use the forward (backward) difference expansion.

2) Solve the same problem with the Full Implicit method. For derivative boundary conditions, use the central difference expansion.

Example: Solve the same equation using the Crank-Nicolson method. For derivative boundary conditions, use the central difference expression.

$$\frac{\partial u}{\partial t}=\frac{\partial^2 u}{(\delta x)^2} \qquad => \qquad \frac{u_{i,j+1}-u_{i,j}}{\delta t}=\frac{1}{2}\frac{u_{i-1,j}-2.u_{i,j}+u_{i+1,j}}{(\delta x)^2}+\frac{1}{2}\frac{u_{i-1,j+1}-2.u_{i,j+1}+u_{i+1,j+1}}{(\delta x)^2}$$

$$-r.u_{i-1,j+1}+(2+2.r).u_{i,j+1}-r.u_{i+1,j+1}=r.u_{i-1,j}+(2-2r).u_{i,j}+r.u_{i+1,j} \qquad (1)$$

$$\frac{\partial u(0,t)}{\partial x}=u(0,t) \qquad => \qquad \frac{u_{1,j}-u_{-1,j}}{2.\delta x}=u_{0,j} \qquad => \qquad u_{-1,j}=u_{1,j}-2.\delta x.u_{0,j} \qquad (2)$$

and $\quad u_{-1,j+1}=u_{1,j+1}-2.\delta x.u_{0,j+1} \qquad (3)$

$$-r.u_{-1,j+1}+(2+2r).u_{0,j+1}-r.u_{1,j+1}=r.u_{-1,j}+(2-2r).u_{0,j}+r.u_{1,j} \qquad (4)$$

if $\delta x=0.1$ is chosen and $r=1$ is taken, when equations (2) and (3) are substituted and arranged in equation (4),

$2.1*u_{0,j+1}-u_{1,j+1}=-0.1*u_{0,j}+u_{1,j}$ for $i=0$,

Equation (1) can be used for the remaining points.

$-u_{i-1,j+1}+4*u_{i,j+1}-u_{i+1,j+1}=u_{i-1,j}+u_{i+1,j}$ $\qquad i=1,2,3,4,5$

If $j=0$,

$$2.1*u_{0,1}-u_{1,1}=-0.1*u_{0,0}+u_{1,0} \qquad i=0$$

$$-u_{0,1}+4*u_{1,1}-u_{2,1}=u_{0,0}+u_{2,0} \qquad i=1$$

$$-u_{1,1}+4*u_{2,1}-u_{3,1}=u_{1,0}+u_{3,0} \qquad i=2$$

$$-u_{2,1}+4*u_{3,1}-u_{4,1}=u_{2,0}+u_{4,0} \qquad i=3$$

$$-u_{3,1}+4*u_{4,1}-u_{5,1}=u_{3,0}+u_{5,0} \qquad i=4$$

$$-u_{4,1}+4*u_{5,1}-u_{6,1}=u_{4,0}+u_{6,0} \qquad i=5$$

When the initial condition is entered,

$$2.1*u_{0,1}-u_{1,1}=-0.1+1.0 \qquad i=0$$

$$-u_{0,1}+4*u_{1,1}-u_{2,1}=1.0+1.0 \qquad i=1$$

$$-u_{1,1}+4*u_{2,1}-u_{3,1}=1.0+1.0 \qquad i=2$$

$$-u_{2,1}+4*u_{3,1}-u_{4,1}=1.0+1.0 \qquad i=3$$

$$-u_{3,1}+4*u_{4,1}-u_{5,1}=1.0+1.0 \qquad i=4$$

$$-u_{4,1}+4*u_{5,1}-u_{6,1}=1.0+1.0 \qquad i=5$$, $u_{6,1}=u_{4,1}$ and $u_{6,0}=u_{4,0}$

If matrix editing is done,

$$2.1*u_0-u_1=-0.1*u_0+u_1=-0.1+1.0 \qquad i=0$$

$$-u_0+4*u_1-u_2=u_0+u_2=1.0+1.0 \qquad i=1$$

$$-u_1+4*u_2-u_3=u_1+u_3=1.0+1.0 \qquad i=2$$

$$-u_2+4*u_3-u_4=u_2+u_4=1.0+1.0 \qquad i=3$$

$$-u_3+4*u_4-u_5=u_3+u_5=1.0+1.0 \qquad i=4$$

$$-u_4+4*u_5-u_4=u_4+u_4=1.0+1.0 \qquad i=5$$

$$
\begin{array}{cccccc}
u_0 & u_1 & u_2 & u_3 & u_4 & u_5
\end{array}
$$

$$
\begin{bmatrix}
2.1 & -1 & 0 & 0 & 0 & 0 \\
-1 & 4 & -1 & 0 & 0 & 0 \\
0 & -1 & 4 & -1 & 0 & 0 \\
0 & 0 & -1 & 4 & -1 & 0 \\
0 & 0 & 0 & -1 & 4 & -1 \\
0 & 0 & 0 & 0 & -2 & 4
\end{bmatrix}
\begin{bmatrix} u_0 \\ u_1 \\ u_2 \\ u_3 \\ u_4 \\ u_5 \end{bmatrix}
=
\begin{bmatrix} -0.1+1.0 \\ 1.0+1.0 \\ 1.0+1.0 \\ 1.0+1.0 \\ 1.0+1.0 \\ 1.0+1.0 \end{bmatrix}
$$

$$
\left.
\begin{aligned}
u_0 &= 0.8908 \\
u_1 &= 0.9707 \\
u_2 &= 0.9922 \\
u_3 &= 0.9979 \\
u_4 &= 0.9994 \\
u_5 &= 0.9997
\end{aligned}
\right\}
$$

For $\delta t = 0.01$,

$r = 1$ and $\delta x = 0.1 = r = \delta t / (\delta x)^2$

If $j = 1$,

$$2.1 * u_0 - u_1 = -0.1 * u_0 + u_1 = -0.08908 + 0.9707 \qquad i = 0$$

$$-u_0 + 4 * u_1 - u_2 = u_0 + u_2 = 0.8908 + 0.9922 \qquad i = 1$$

$$-u_1 + 4 * u_2 - u_3 = u_1 + u_3 = 0.9707 + 0.9979 \qquad i = 2$$

$$-u_2 + 4 * u_3 - u_4 = u_2 + u_4 = 0.9922 + 0.9994 \qquad i = 3$$

$$-u_3 + 4 * u_4 - u_5 = u_3 + u_5 = 0.9979 + 0.9997 \qquad i = 4$$

$$-u_4 + 4 * u_5 - u_6 = u_4 + u_6 = 0.9994 + 0.9994 \qquad i = 5$$

$$
\begin{array}{c}
\begin{array}{cccccc} u_0 & u_1 & u_2 & u_3 & u_4 & u_5 \end{array} \\
\begin{bmatrix} 2.1 & -1 & 0 & 0 & 0 & 0 \\ -1 & 4 & -1 & 0 & 0 & 0 \\ 0 & -1 & 4 & -1 & 0 & 0 \\ 0 & 0 & -1 & 4 & -1 & 0 \\ 0 & 0 & 0 & -1 & 4 & -1 \\ 0 & 0 & 0 & 0 & -2 & 4 \end{bmatrix}
\end{array}
\begin{bmatrix} u_0 \\ u_1 \\ u_2 \\ u_3 \\ u_4 \\ u_5 \end{bmatrix} = \begin{bmatrix} -0.08908+09707 \\ 0.8908+0.9922 \\ 0.9707+0.9979 \\ 0.9922+0.9994 \\ 0.9979+0.9997 \\ 0.9994+0.9994 \end{bmatrix}
$$

	$i=0$ $x=0$	$i=1$ $x=0.1$	$i=2$ $x=0.2$	$i=3$ $x=0.3$	$i=4$ $x=0.4$	$i=5$ $x=0.5$
$t=0.000$	1.0	1.0	1.0	1.0	1.0	1.0
$t=0.01$	0.8908	0.9707	0.9922	0.9979	0.9994	0.9997
$t=0.02$	0.8624	0.9293	0.9720	0.9900	0.9964	0.9979
.	.	.	.	.	.	.
.	.	.	.	.	.	.
.	.	.	.	.	.	.
$t=0.10$	0.7179	0.7834	0.8349	0.8720	0.8944	0.9018
$t=0.25$	0.5547	0.6054	0.6458	0.6751	0.6929	0.6989
$t=0.50$	0.3618	0.3949	0.4212	0.4404	0.4520	0.4559
$t=1.00$	0.1540	0.1680	0.1793	0.1874	0.1923	0.1940

NOT: $\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + 2x\frac{\partial u}{\partial x} + u + x$

When the equation is opened with Crank-Nicolson, the values other than the second derivative become:

$$
\ldots = \ldots + 2.x_i\left[\frac{1}{2}\frac{u_{i+1,j} - u_{i-1,j}}{2.\delta x} + \frac{1}{2}\frac{u_{i+1,j+1} - u_{i-1,j+1}}{2.\delta x}\right] + \left[\frac{1}{2}u_{i,j} + \frac{1}{2}u_{i,j+1}\right] + x_i
$$

7.5. Convergence and Stability

It is very difficult to estimate the accuracy of the results of finite difference equations. However, if the two criteria known as convergence and stability are met, accuracy can be achieved by increasing the number of steps and thus increasing the number of operations.

If the time and size steps goes to "0", the approximate numerical solution converges to the analytical solution, the solution is said to be convergent. If the numerical method converges to the analytical solution in the limit, it can be said that the method has achieved the convergence criterion.

When the differential equation and boundary conditions are written as a finite difference equation, operations are performed for a finite number of time and dimension steps. Rounding errors are also processed during these operations. If these errors do not grow as the solution progresses, it can be said that the solution is stable. Stability is also a necessary condition for convergence in reality.

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}$$

=> $$\frac{u_{i,j+1} - u_{i,j}}{\delta t} + O(\delta t) = \frac{u_{i-1,j} - 2 * u_{i,j} + u_{i+1,j}}{(\delta x)^2} + O(\delta x)^2$$

1- the finite difference equation cannot be represented

2- rounding error

$u_{i,j+1} = r.u_{i-1,j} + (1-2r).u_{i,j} + r.u_{i+1,j}$ and $r = \frac{\delta t}{(\delta x)^2}$

At any instant t, the solution can be expanded to the Fourier series. If we neglect the constants, the general term of solution of the differential equation will be in the form of

$u(x,t)=\phi(t).e^{\hat{\imath}.\beta.x}$. By substituting this expression in the finite difference equation, $\phi(t)$ can be determined, and as t gets larger, the criterion for $\phi(t)$ to be limited can be determined.

$\hat{\imath}=\sqrt{-1}$ and $e^{\hat{\imath}.\beta.x}=\cos\beta.x+\hat{\imath}.\sin\beta.x$

As time progresses $\left|\dfrac{\phi(t+\delta t)}{\phi(t)}\right|\le 1$ must be (convergence condition).

$$u_{i,j}=\phi(t).e^{\hat{\imath}\beta.x}$$

$$u_{i-1,j}=\phi(t).e^{\hat{\imath}\beta.(x-\delta x)}$$

$$u_{i+1,j}=\phi(t).e^{i\beta.(x+\delta x)}$$

$$u_{i,j+1}=\phi(t+\delta t).e^{\hat{\imath}\beta.x}$$

Substituting these in the finite difference equation expression, we get

$$\phi(t+\delta t).e^{\hat{\imath}\beta.x}=r.\phi(t).e^{\hat{\imath}\beta.(x-\delta x)}+(1-2r).\phi(t).e^{\hat{\imath}\beta.x}+r.\phi(t).e^{\hat{\imath}\beta.(x+\delta x)}$$

If we divide both sides by $\phi(t).e^{\hat{\imath}\beta.x}$ expression,

$$\frac{\phi(t+\delta t)}{\phi(t)}=r.e^{-\hat{\imath}.\beta.\delta x}+(1-2r)+r.e^{\hat{\imath}.\beta.\delta x}$$

$$e^{\hat{\imath}.\beta.\delta x}=\cos\beta.\delta x+\hat{\imath}.\sin\beta.\delta x$$

$$e^{-\hat{\imath}.\beta.\delta x}=\cos\beta.\delta x-\hat{\imath}.\sin\beta.\delta x$$

=> $e^{\hat{\imath}.\beta.\delta x}+e^{-\hat{\imath}.\beta.\delta x}=2.\cos\beta.\delta x$

=> $=(1-2r)+r.\left(e^{-\hat{\imath}.\beta.\delta x}+e^{\hat{\imath}.\beta.\delta x}\right)$

=> $=(1-2r)+r.(2.\cos\beta.\delta x)$

If we arrange,

$$\frac{\phi(t+\delta t)}{\phi(t)} = 1-4r\left[\frac{1-\cos\beta.\delta x}{2}\right] \qquad \text{and} \qquad \frac{1-\cos\beta.\delta x}{2} = \sin^2\frac{\beta.\delta x}{2}$$

=> $= 1-4r.\sin^2\dfrac{\beta.\delta x}{2}$

For stability, the value of $\phi(t)$ should be limited as δx and δt go to 0.

$$\left|\frac{\phi(t+\delta t)}{\phi(t)}\right| \le 1 \qquad \Rightarrow \qquad \left|1-4r.\sin^2\frac{\beta.\delta x}{2}\right| \le 1$$

($\sin^2\dfrac{\beta.\delta x}{2} = 1$), maximum value it can take

$|1-4r| \le 1$ in other words $-1 \le 1-4.r \le 1$

=> $0 \le r$ and $r \le \dfrac{1}{2}$ has a range.

$r = \dfrac{\delta t}{(\delta x)^2}$ Explicit method is therefore not used.

This approach is called the *Von Neumann* approach.

The term with $\phi(t)$ should not go to ∞ and take a limited value.

7.6. Formulation of Two-Dimensional Unsteady (Time-Dependent) Heat Transfer Problems in Cartesian Coordinates

$$\frac{\partial u}{\partial t}=\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 u}{\partial y^2}$$

$$u(x,y,t)\rightarrow u_{m,n}^{A}$$

$A\rightarrow f(t)$, $m\rightarrow f(x)$, $n\rightarrow f(y)$

$$\frac{u_{m,n}^{A+1}-u_{m,n}^{A}}{\delta t}=\frac{u_{m-1,n}^{A}-2.u_{m,n}^{A}+u_{m+1,n}^{A}}{(\delta x)^2}+\frac{u_{m,n-1}^{A}-2.u_{m,n}^{A}+u_{m,n+1}^{A}}{(\delta y)^2} \quad \text{(Explicit)}$$

$r_1=\dfrac{\delta t}{(\delta x)^2}$ $\qquad$ $r_2=\dfrac{\delta t}{(\delta y)^2}$ $\qquad$ $r_1, r_2\le\dfrac{1}{4}$

If a fully implicit solution is desired, the A's on the right side of the equation become $(A+1)$.

7.7. Formulation of Unsteady (Time Dependent) Heat Transfer Problems in Cylindrical Coordinates

$$\frac{\partial u}{\partial t}=\nabla^2 u$$

$$\frac{\partial u}{\partial t}=\frac{\partial^2 u}{\partial r^2}+\frac{1}{r}\frac{\partial u}{\partial r}+\frac{1}{r^2}\frac{\partial^2 u}{\partial \theta^2}+\frac{\partial^2 u}{\partial z^2} \qquad u(r,\theta,z,t)\rightarrow u_{m,n,k}^{A}$$

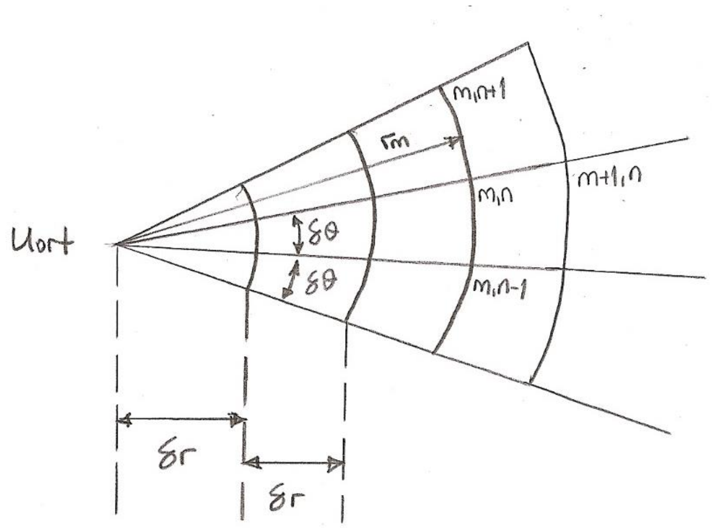
$A\rightarrow f(t)$, $m\rightarrow f(r)$, $n\rightarrow f(\theta)$, $k\rightarrow f(z)$

$$\frac{u_{m,n,k}^{A+1}-u_{m,n,k}^{A}}{\delta t}=\frac{u_{m-1,n,k}^{A}-2.u_{m,n,k}^{A}+u_{m+1,n,k}^{A}}{(\delta r)^2}+\frac{1}{r_m}\frac{u_{m+1,n,k}^{A}-u_{m-1,n,k}^{A}}{2.\delta r}+$$

$$+\frac{1}{r_m^2}\frac{u_{m,n-1,k}^A-2.u_{m,n,k}^A+u_{m,n+1,k}^A}{(\delta\theta)^2}+\frac{u_{m,n,k-1}^A-2.u_{m,n,k}^A+u_{m,n,k+1}^A}{(\delta z)^2} \quad \text{(Explicit)}$$

$$r_m=m.\delta r$$

If a fully implicit solution is desired, the A's on the right side of the equation become $(A+1)$.



Here u_{ort} is the weighted average of the temperatures at the lattice points surrounding $r=0$. (Because at $r=0$ the equation is unsolvable)

$$\frac{\partial u}{\partial t}=2.x^2\frac{\partial^2 u}{\partial x^2}+\frac{\partial u}{\partial x}+x^2.u$$

$$=> \quad \frac{u_{i,j+1}-u_{i,j}}{\delta t}=2.x_i^2\frac{u_{i-1,j}-2.u_{i,j}+u_{i+1,j}}{(\delta x)^2}+\frac{u_{i+1,j}-u_{i-1,j}}{2.\delta x}+x_i^2.u_{i,j} \quad \text{(Explicit)}$$

If a fully implicit solution is desired, the A's on the right side of the equation become $(A+1)$.

8. HYPERBOLIC EQUATIONS

8.1. Explicit Method and Courant-Friedrichs-Lewy Condition

The wave equation is a hyperbolic equation.

$$\frac{\partial^2 u}{\partial t^2} = \frac{\partial^2 u}{\partial x^2}$$

$u(x,t) = u_{i,j}$ and $i \to x$, $j \to t$

$$\left.\begin{aligned} &u(x,0) = f(x) \\ &\frac{\partial u(x,0)}{\partial t} = g(x) \end{aligned}\right\} \quad \text{Initial conditions for } t = 0$$

$$\left.\begin{aligned} &u(0,t) = 0 \\ &u(1,t) = 0 \end{aligned}\right\} \quad \text{It is homogenous, If it is "}a\text{" and "}b\text{",}$$

When an analytical solution is desired, we can write $v(x,t) = u(x,t) - a + (a-b).x$

$$\frac{u_{i,j-1} - 2.u_{i,j} + u_{i,j+1}}{(\delta t)^2} = \frac{u_{i-1,j} - 2.u_{i,j} + u_{i+1,j}}{(\delta x)^2}$$

if arranged,

$$u_{i,j+1} = r^2.u_{i-1,j} + 2.(1-r^2).u_{i,j} + r^2.u_{i+1,j} - u_{i,j-1} \tag{1}$$

$$r = \frac{\delta t}{\delta x}$$

$$u_{i,1} = r^2.u_{i-1,0} + 2.(1-r^2).u_{i,0} + r^2.u_{i+1,0} - u_{i,-1} \tag{2}$$

Initial conditions,

$u(x,0) = f(x)$ => $u_{i,0} = f_i$

$\dfrac{\partial u(x,0)}{\partial t} = g(x)$ => $\dfrac{u_{i,1} - u_{i,-1}}{2.\delta t} = g_i$

=> $u_{i,-1} = u_{i,1} - 2.\delta t.g_i$

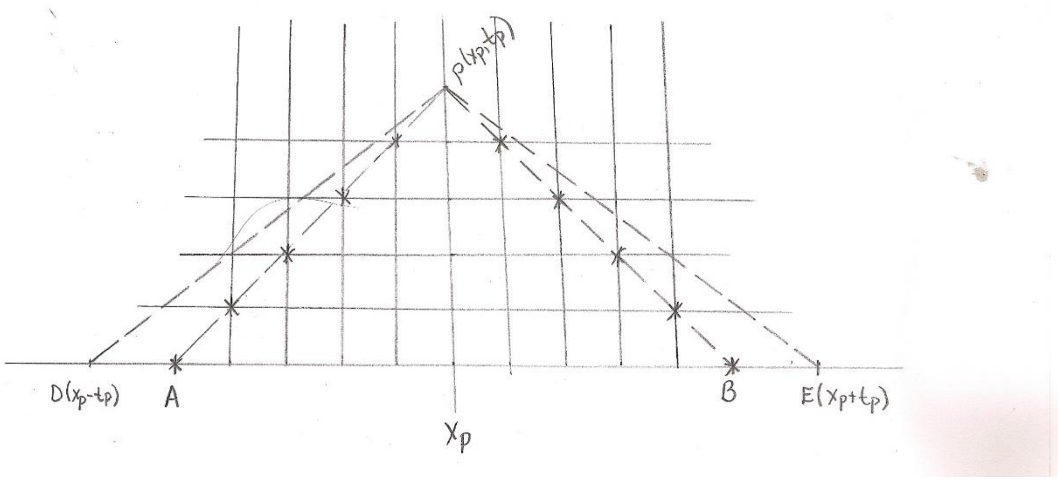
If we substitute it in equation (2),

$$u_{i,1} = r^2.u_{i-1,0} + 2.(1-r^2).u_{i,0} + r^2.u_{i+1,0} - (u_{i,1} - 2.\delta t.g_i)$$

$$u_{i,1} = \frac{1}{2}\left\{r^2.u_{i-1,0} + 2.(1-r^2).u_{i,0} + r^2.u_{i+1,0} + 2.\delta t.g_i\right\} \tag{3}$$

Analytical solution of the wave equation by D'Alembert is that

$$u(x,t) = \frac{1}{2}\left\{ f(x+t) + f(x-t) + \int_{x-t}^{x+t} g(\xi).d\xi \right\}$$



If the wave equation is solved numerically with the help of equations (1) and (3), $u_{i,j}$ value at the P point will depend on the value of the remaining lattice points within the ABP. Suppose the initial conditions in DA and BE are changed. Although the change made in these initial conditions changes the analytical solution result in P, the numerical solution value at the point P found with the help of equations (1) and (3) will not change. In this case, the numerical solution will not converge to the analytical solution. Then the value of $r=\dfrac{\delta t}{\delta x}$ should be chosen such that while there is a numerical solution at the point P, the initial conditions between DE should also reflect the solution.

This condition, known as the Courant-Frendrich-Lewy condition, is $r=\dfrac{\delta t}{\delta x}$. Usually $r=1$ is taken.

Example: Solve the $\dfrac{\partial^2 u}{\partial t^2}=\dfrac{\partial^2 u}{\partial x^2}$ equation.

$$\left.\begin{aligned} u(x,0) &= \frac{1}{8}\sin \pi .x = f(x) \\ \frac{\partial u(x,0)}{\partial t} &= 0 = g(x) \end{aligned}\right\} \quad \text{Initial conditions } (t=0)$$

$$\left.\begin{aligned} u(0,t) &= 0 \\ u(1,t) &= 0 \end{aligned}\right\} \quad \text{Boundary conditions } (t>0)$$

$\delta x=\dfrac{1-0}{10}=0.1$ (divided into 10 parts) $\quad r=\dfrac{\delta t}{\delta x}=1 \quad$ => $\quad \delta t=0.1$ becomes

$$u_{i,j+1} = u_{i-1,j} + u_{i+1,j} - u_{i,j-1} \qquad (1)$$

$$u_{i,1} = \frac{1}{2}\left\{u_{i-1,0} + u_{i+1,0} + 2.\delta t.g_{i,0}\right\} \qquad g_{i,0} = 0 \qquad (2)$$

$$u_{i,1} = \frac{1}{2}\left\{u_{i-1,0} + u_{i+1,0}\right\} \qquad (3)$$

$u_{i,0} = f_i = \frac{1}{8}\sin \pi.x_i$ => $u_{i,0} = \frac{1}{8}\sin(0.1*\pi*i)$

$x_i = x_0 + i.\delta x$ => $x_i = 0.1*i$

$u_{0,0} = 0$

$u_{1,0} = \frac{1}{8}\sin(0.1*\pi) = 0.03863$

$u_{2,0} = \frac{1}{8}\sin(0.2*\pi) = 0.07347$

$u_{3,0} = 0.10113$

$u_{4,0} = 0.1189$

$u_{5,0} = 0.125$

$u_{6,0} = 0.1189$

$u_{7,0} = 0.10113$ (Since there is symmetry in the values, it will be sufficient to solve for half of the wire.)

	$i=0$ $x=0$	$i=1$ $x=0.1$	$i=2$ $x=0.2$	$i=3$ $x=0.3$	$i=4$ $x=0.4$	$i=5$ $x=0.5$	......	$i=10$ $x=1.0$	
$t=0.0$	0.0	0.03863	0.07347	0.1013	0.1189	0.125	......	0.0	İnitial condition
$t=0.1$	0.0	0.0367	0.0699	0.0962	0.1131	0.1189	......	0.0	From Eq. (3)

$t = 0.2$	0.0	0.0312	0.0594	0.0818	0.0962	0.1011	......	0.0	
$t = 0.3$	0.0	0.0227	0.0432	0.0594	0.0699	0.0735	......	0.0	From Eq. (1)
$t = 0.4$	0.0	0.0119	0.0227	0.0312	0.0368	0.0386	......	0.0	
$t = 0.5$	0.0	0.0	0.0	0.0	0.0	0.0	......	0.0	
$t = 0.6$	0.0	-.0119	-.0227	-.0312	-.0368	-.0386	......	0.0	
Analytical Solution $t = 0.3$	0.0	0.0227	0.0432	0.0594	0.0699	0.0735	......	0.0	

Analytical Solution: $u = \frac{1}{8}\sin\pi.x * \cos\pi.t$

In the first step, we use equation (3). Then we find the solution using other equations.

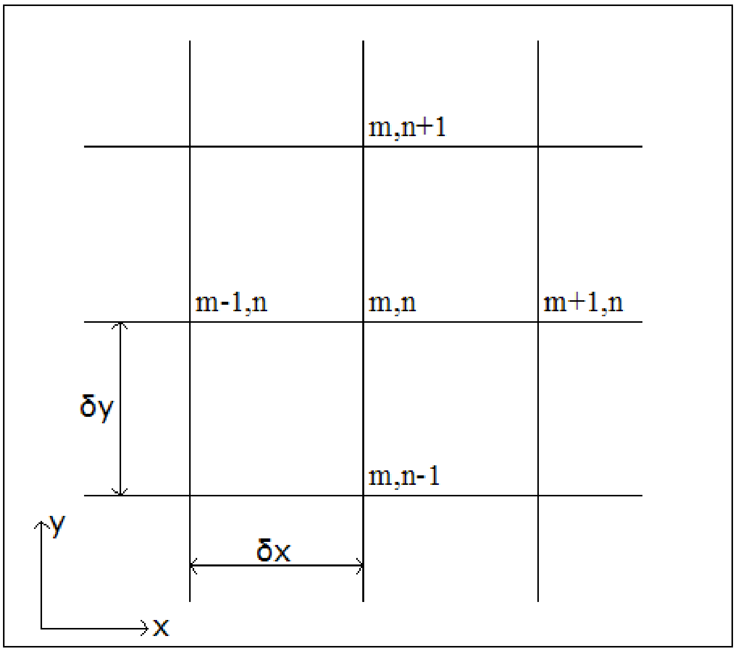
9. ELLIPTICAL EQUATIONS

9.1. Formulation and Solution of Heat Conduction Equation in Steady State in Cartesian Coordinates

$$\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} = 0$$

$T(x, y) \to T_{m,n}$ $\qquad$ $m \to f(x)$ $\qquad$ $n \to f(y)$

$$\frac{T_{m-1,n} - 2.T_{m,n} + T_{m+1,n}}{(\delta x)^2} + \frac{T_{m,n-1} - 2.T_{m,n} + T_{m,n+1}}{(\delta y)^2} = 0$$



If $\delta x = \delta y$,

$$T_{m-1,n} + T_{m+1,n} + T_{m,n-1} + T_{m,n+1} = 4.T_{m,n}$$

$$\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\bar{q}}{k} = 0$$

=> $$\frac{T_{m-1,n} - 2.T_{m,n} + T_{m+1,n}}{(\delta x)^2} + \frac{T_{m,n-1} - 2.T_{m,n} + T_{m,n+1}}{(\delta y)^2} + \frac{\bar{q}}{k} = 0$$ and $\bar{q} \rightarrow \left(\frac{W}{m^2}\right)$

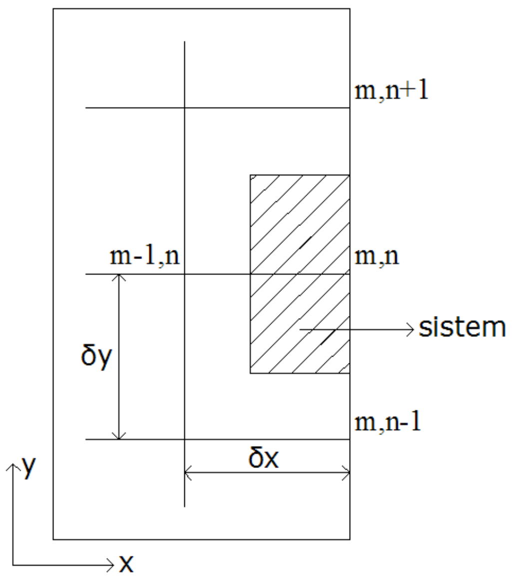
İf $\delta x = \delta y$,

$$T_{m-1,n} + T_{m+1,n} + T_{m,n-1} + T_{m,n+1} + \frac{\bar{q}}{k}(\delta x)^2 = 4.T_{m,n}$$

9.2. Boundary Conditions

We have obtained the finite difference equation for the two-dimensional system. This equation is valid for every node of the lattice inside the rigid body. The boundary conditions must be known to calculate the boundary temperatures as they approach the boundary. Let us now examine how the boundary conditions are written in terms of finite differences.

9.2.1. The Boundary Condition for Given Fluid Temperature and Film Coefficient



T∞ : Akiskanin Sicakligi

h : Akiskanin Film Katsayisi

Thickness of Solid : b

Fourier's Law of Heat Conduction : $Q = -k.A.\dfrac{dT}{dn}$

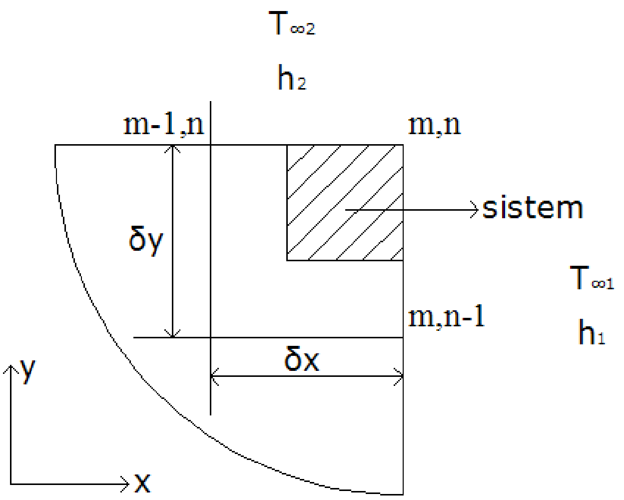
Newton's Law of Cooling : $Q = h.A.(T - T_\infty)$

$$-k.\delta y.b\frac{T_{m,n} - T_{m-1,n}}{\delta x} - k\frac{\delta x}{2}b\frac{T_{m,n} - T_{m,n-1}}{\delta y} - k\frac{\delta x}{2}b\frac{T_{m,n} - T_{m,n+1}}{\delta y} = h.b.\delta y.(T_{m,n} - T_\infty)$$

If $\delta x = \delta y$,

$$\frac{1}{2}(2.T_{m-1,n} + T_{m,n-1} + T_{m,n+1}) + \frac{h.\delta x}{k}T_\infty - T_{m,n}\left(\frac{h.\delta x}{k} + 2\right) = 0$$

If the boundary consists of a corner, as shown in the figure below, the heat conduction law, together with the Fourier and Newton rules, can be applied to the system shown in the figure,



$$-k.\frac{\delta y}{2}.b\frac{T_{m,n} - T_{m-1,n}}{\delta x} - k\frac{\delta x}{2}b\frac{T_{m,n} - T_{m,n-1}}{\delta y} = h_1\frac{\delta y}{2}b(T_{m,n} - T_{\infty 1}) + h_2\frac{\delta x}{2}b(T_{m,n} - T_{\infty 2})$$

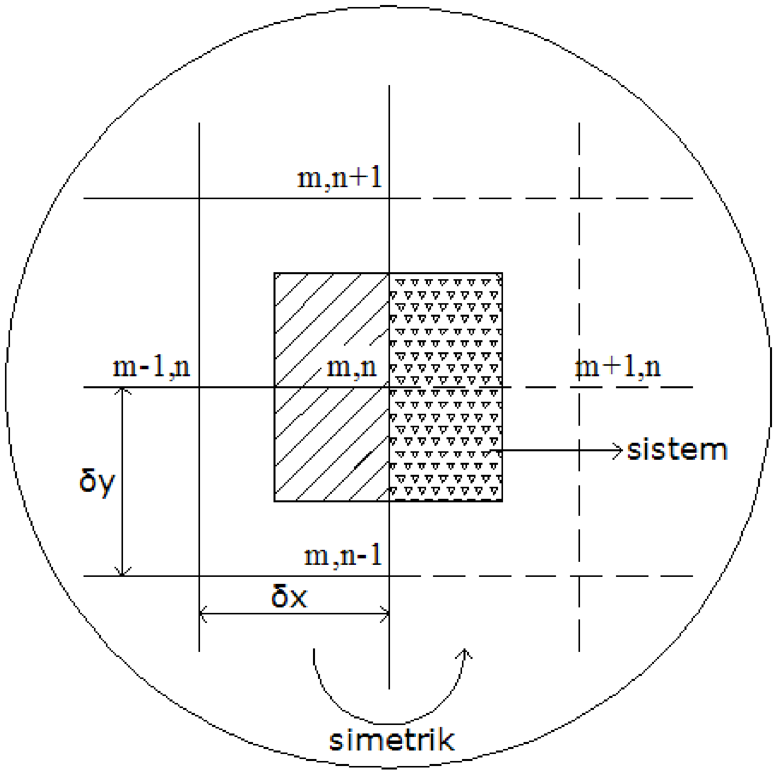
If the variable expressing the thickness of the solid body is eliminated on both sides of the equation, the system of equations takes its final form.

9.2.2. Given Boundary Temperature

This is used exactly as the temperatures are given at the boundary.

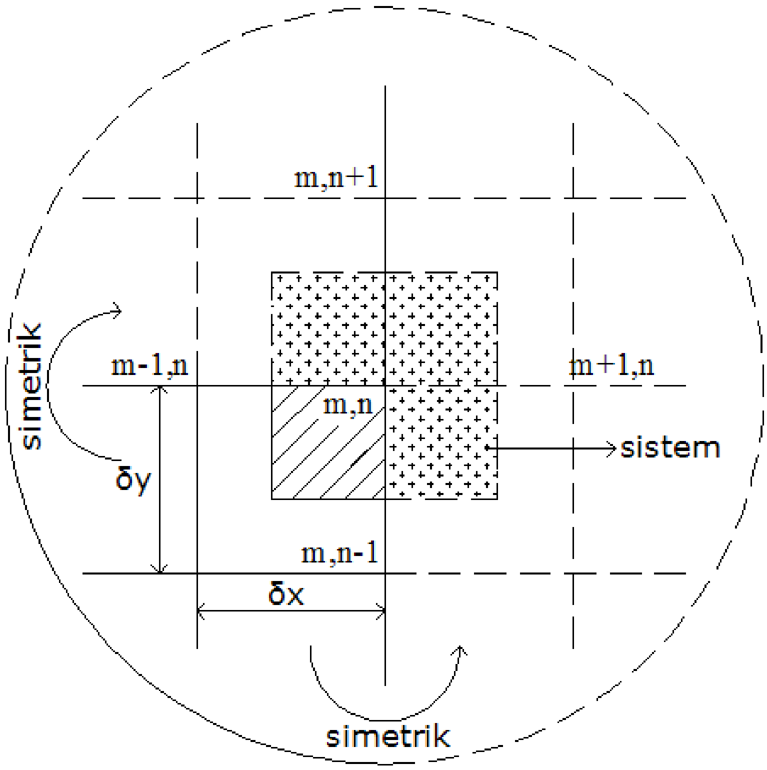
9.2.3. Isolated border

It is assumed that there is no heat transfer from the boundary.



$$-k.\delta y.b\frac{T_{m,n}-T_{m-1,n}}{\delta x}-k.\delta y.b\frac{T_{m,n}-T_{m-1,n}}{\delta x}-k.\delta x.b\frac{T_{m,n}-T_{m,n-1}}{\delta y}-k.\delta x.b\frac{T_{m,n}-T_{m,n+1}}{\delta y}=0$$

In systems with isolated boundary conditions, the solution can be made by taking the symmetry of the system. as well as the expression found in "The Boundary Condition for Given Fluid Temperature and Film Coefficient" case, the film coefficient " h " can be set to " 0 ", the equation is obtained.

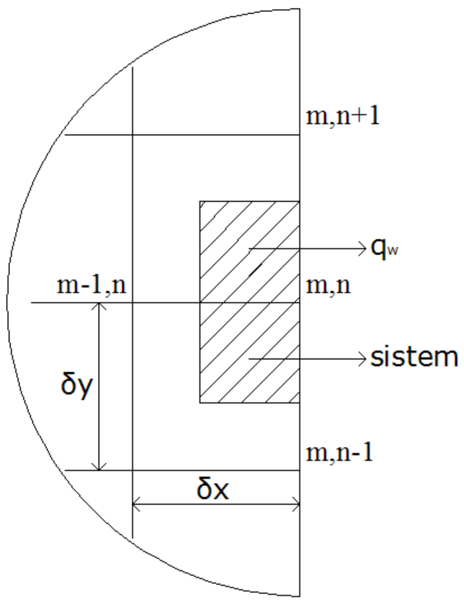


In this case, the general heat conduction equation becomes:

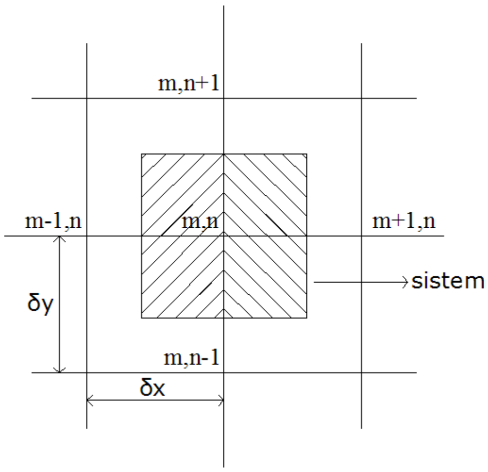
$$-k\frac{\delta y}{2}\frac{T_{m,n}-T_{m-1,n}}{\delta x}-k\frac{\delta x}{2}\frac{T_{m,n}-T_{m,n-1}}{\delta y}=0$$

9.2.4. Given Boundary Heat Flux

If the heat flux is given at the boundary, the expression $q_w.\delta y.b$ is put in place of the last term in the expression obtained for the boundary where the film coefficient is given. Here, q_w is the heat flux from the system to outer space.



Example:

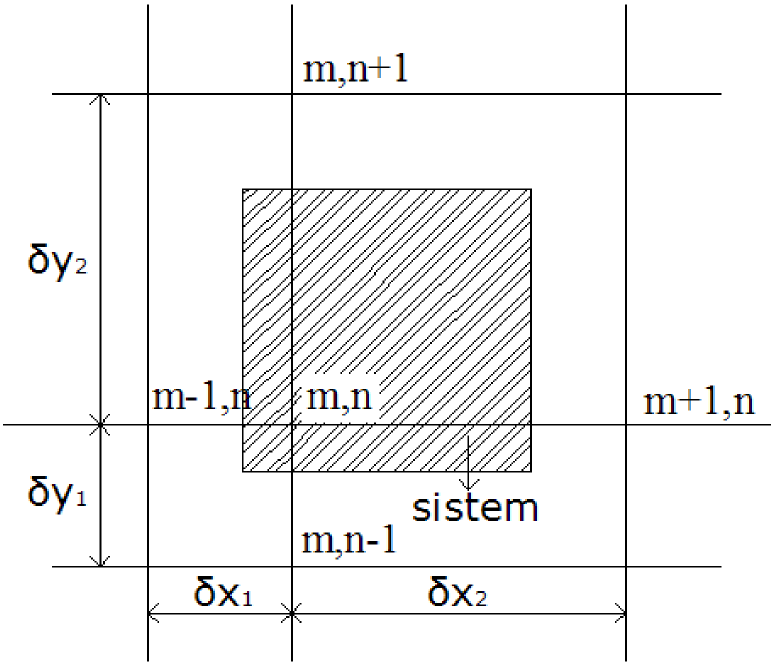


$$-k.\delta y.b\frac{T_{m,n}-T_{m-1,n}}{\delta x}-k.\delta y.b\frac{T_{m,n}-T_{m+1,n}}{\delta x}-k.\delta x.b\frac{T_{m,n}-T_{m,n-1}}{\delta y}-k.\delta x.b\frac{T_{m,n}-T_{m,n+1}}{\delta y}=0$$

If the variables k and b are eliminated and the equality divided by $\delta x.\delta y$,

$$\frac{T_{m-1,n} - 2.T_{m,n} + T_{m+1,n}}{(\delta x)^2} + \frac{T_{m,n-1} - 2.T_{m,n} + T_{m,n+1}}{(\delta y)^2} = 0 \qquad \Leftarrow \qquad \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} = 0$$

Example:

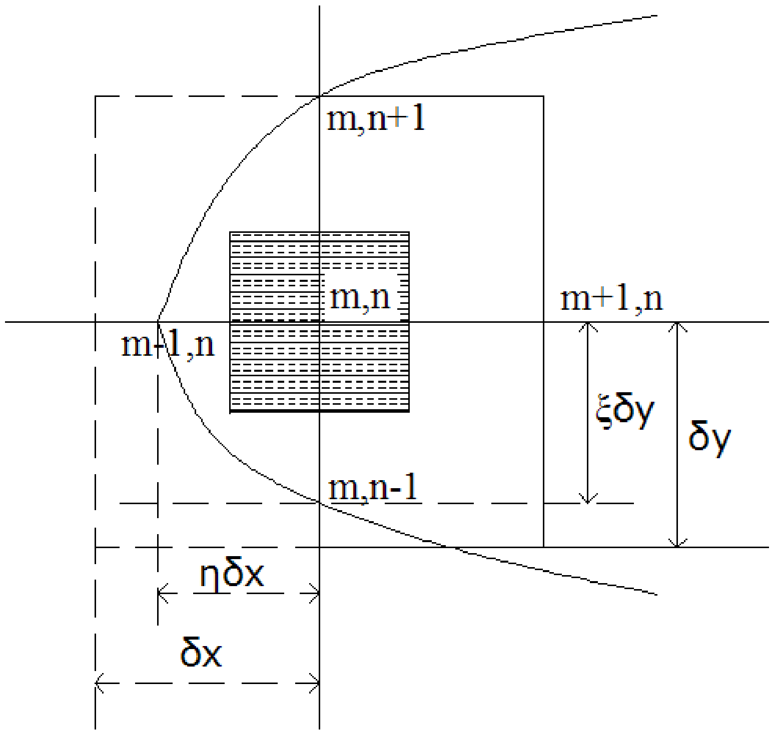


$$-k.\left(\frac{\delta y_1 + \delta y_2}{2}\right).b\,\frac{T_{m,n} - T_{m-1,n}}{\delta x_1} - k.\left(\frac{\delta y_1 + \delta y_2}{2}\right).b\,\frac{T_{m,n} - T_{m+1,n}}{\delta x_2}$$

$$-k.\left(\frac{\delta x_1 + \delta x_2}{2}\right).b\,\frac{T_{m,n} - T_{m,n-1}}{\delta y_1} - k.\left(\frac{\delta x_1 + \delta x_2}{2}\right).b\,\frac{T_{m,n} - T_{m,n+1}}{\delta y_2} = 0$$

9.3. Curved Borders

The main benefit of the finite difference method is that it can also be used for complex boundaries. If the boundaries of a solid body are not parallel to the coordinate axis,



Dimensions of the system,

$$\left(\frac{\delta x}{2}+\frac{\eta.\delta x}{2}\right)=\frac{\delta x}{2}(1+\eta)$$

$$\left(\frac{\delta y}{2}+\frac{\xi.\delta y}{2}\right)=\frac{\delta y}{2}(1+\xi)$$

$$-k.\frac{\delta y}{2}(1+\xi).b\frac{T_{m,n}-T_{m-1,n}}{\eta.\delta x}-k.\frac{\delta y}{2}(1+\xi).b\frac{T_{m,n}-T_{m+1,n}}{\delta x}$$

$$-k.\frac{\delta x}{2}(1+\eta).b\frac{T_{m,n}-T_{m,n-1}}{\xi.\delta y}-k.\frac{\delta x}{2}(1+\eta).b\frac{T_{m,n}-T_{m,n+1}}{\delta y}=0$$

If $\delta x=\delta y$,

$$\frac{2}{(1+\xi)}T_{m,n+1} + \frac{2}{(1+\eta)}T_{m+1,n} + \frac{2}{\xi.(1+\xi)}T_{m,n-1} + \frac{2}{\eta.(1+\eta)}T_{m-1,n} - \left(\frac{2}{\eta} + \frac{2}{\xi}\right).T_{m,n} = 0$$

If $\eta = 1$ and $\xi = 1$,

$T_{m,n+1} + T_{m+1,n} + T_{m,n-1} + T_{m-1,n} - 4.T_{m,n} = 0$ (general formula)

10. GAUSS-SEIDEL POINT BY POINT ITERATION METHOD

It is the simplest of the iteration methods, and the calculation is made by considering the variable values at each grid point. If the finite difference equation for the grid point " P " is given as follows,

$$a_p.T_p = \sum a_{nb}.T_{nb} + b$$

Here, the index nb denotes neighboring points.

$$4.T_{m,n} = 3.T_{m-1,n} + 2.T_{m+1,n} + 8.T_{m,n-1} + 3T_{m,n+1} + K \text{ (Example)}$$

$$T_p = \frac{\sum a_{nb}.T^*_{nb} + b}{a_p}$$

T^*_{nb}, are the values of neighboring points before iteration or the first estimated values. For each lattice point, new values can be found with the above equation. Iteration is continued until the difference between the iterations is less than a certain ε.

Example: $T_1 = 0.4 * T_2 + 0.2$

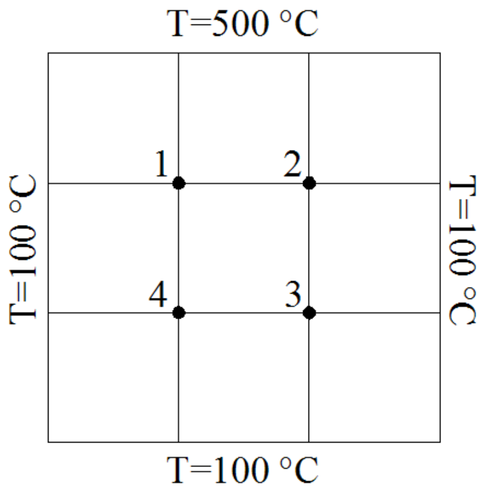
$T_2 = T_1 + 1.0$, Find the T_1 and T_2 values using the Gauss-Seidel iteration method.

Iteration No	0	1	2	3	4	5	...	∞
T_1	0 (initial prediction)	0.2	0.68	0.872	0.949	0.98	...	1

T_2	0 (initial prediction)	1.2	1.68	1.872	1.949	1.98	...	2

As the iteration continues, the last values that emerged in the iteration are used.

Example: Find the temperature distribution in the solid body under the boundary conditions given in the figure, using the Gauss-Seidel iteration method. ($\delta x = \delta y$)



$$4.T_1 = 100 + 500 + T_2 + T_4$$
$$4.T_2 = 500 + 100 + T_1 + T_3$$
$$4.T_3 = T_2 + T_4 + 100 + 100$$
$$4.T_4 = 100 + T_1 + T_3 + 100$$

$$T_1 = \frac{T_2 + T_4}{4} + 150 \qquad T_2 = \frac{T_1 + T_3}{4} + 150$$

$$T_3 = \frac{T_2 + T_4}{4} + 50 \qquad T_4 = \frac{T_1 + T_3}{4} + 50$$

Iteration No	0 (initial prediction)	1	2	3	...	∞
T_1	300	275	257,33	252,25	...	250
T_2	300	268,75	256,13	251,61	...	250
T_3	200	167,19	154,17	151,12	...	150
T_4	200	160,55	152,88	150,84	...	150

The Gauss-Seidel method does not always converge, it is sufficient to meet the Scarborough criterion for convergence.

Scarborough criterion ; $$\frac{\sum |a_{nb}|}{|a_p|} \begin{cases} \leq 1 & \text{for all equations} \\ < 1 & \text{for at least one equation} \end{cases}$$

For example, $T_1 = 0.4 * T_2 + 0.2 \Rightarrow \frac{0.4}{1}$ and $T_2 = T_1 + 1.0 \Rightarrow \frac{1.0}{1.0}$ satisfies Scarborough criterion

But if we change the order of equations,

$T_1 = T_2 - 1.0 \Rightarrow \frac{1.0}{1.0}$ and $T_2 = 2.5 * T_1 - 0.5 \Rightarrow \frac{2.5}{1.0} = 2.5$ does not satisfy Scarborough criterion.

Iteration No	0	1	2	3
T_1	0	-1	-4	-11.5
T_2	0	-3	-10.5	...