MATHEMATICAL METHODS

NUMERICAL DIFFERENTIATION & INTEGRATION

I YEAR B.Tech

AS PER JNTU-HYDERABAD NEW SYLLABUS

By

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SYLLABUS OF MATHEMATICAL METHODS (as per JNTU Hyderabad)

Name of the Unit	Name of the Topic
Unit-I **Solution of Linear systems**	**Matrices and Linear system of equations:** Elementary row transformations – Rank – Echelon form, Normal form – Solution of Linear Systems – Direct Methods – LU Decomposition from Gauss Elimination – Solution of Tridiagonal systems – Solution of Linear Systems.
Unit-II **Eigen values and Eigen vectors**	Eigen values, Eigen vectors – properties – Condition number of Matrix, Cayley – Hamilton Theorem (without proof) – Inverse and powers of a matrix by Cayley – Hamilton theorem – Diagonalization of matrix – Calculation of powers of matrix – Model and spectral matrices.
Unit-III **Linear Transformations**	Real Matrices, Symmetric, skew symmetric, Orthogonal, Linear Transformation - Orthogonal Transformation. Complex Matrices, Hermition and skew Hermition matrices, Unitary Matrices - Eigen values and Eigen vectors of complex matrices and their properties. Quadratic forms - Reduction of quadratic form to canonical form, Rank, Positive, negative and semi definite, Index, signature, Sylvester law, Singular value decomposition.
Unit-IV **Solution of Non-linear Systems**	**Solution of Algebraic and Transcendental Equations-** Introduction: The Bisection Method – The Method of False Position – The Iteration Method - Newton –Raphson Method **Interpolation:**Introduction-Errors in Polynomial Interpolation - Finite differences- Forward difference, Backward differences, Central differences, Symbolic relations and separation of symbols-Difference equations – Differences of a polynomial - Newton's Formulae for interpolation - Central difference interpolation formulae - Gauss Central Difference Formulae - Lagrange's Interpolation formulae- B. Spline interpolation, Cubic spline.
Unit-V **Curve fitting & Numerical Integration**	**Curve Fitting:** Fitting a straight line - Second degree curve - Exponential curve - Power curve by method of least squares. **Numerical Integration:** Numerical Differentiation-Simpson's 3/8 Rule, Gaussian Integration, Evaluation of Principal value integrals, Generalized Quadrature.
Unit-VI **Numerical solution of ODE**	Solution by Taylor's series - Picard's Method of successive approximation- Euler's Method -Runge kutta Methods, Predictor Corrector Methods, Adams- Bashforth Method.
Unit-VII **Fourier Series**	Determination of Fourier coefficients - Fourier series-even and odd functions - Fourier series in an arbitrary interval - Even and odd periodic continuation - Half-range Fourier sine and cosine expansions.
Unit-VIII **Partial Differential Equations**	Introduction and formation of PDE by elimination of arbitrary constants and arbitrary functions - Solutions of first order linear equation - Non linear equations - Method of separation of variables for second order equations - Two dimensional wave equation.

CONTENTS

UNIT-V

NUMERICAL DIFFERENTIATION & INTEGRATION

Numerical Differentiation and Integration

Numerical Differentiation

$$x \quad : \quad x_0 \quad x_1 \quad x_2 \quad \dots \quad x_n \longrightarrow \text{Equally Spaced Arguments}$$

$$y = f(x) : \quad f_0 \quad f_1 \quad f_2 \quad \dots \quad f_n$$

Aim: We want to calculate $\frac{dy}{dx}, \frac{d^2y}{dx^2}, \frac{d^3y}{dx^3}, \dots$ at the tabulated points.

The intention of Using these formulas is that, without finding the polynomial for the given curve, we will find its first, second, third, . . . derivatives.

Since Arguments are equally spaced, we can use Forward, Backward or Central differences.

Differentiation using Forward Differences

We know that $\Delta f(x) = f(x+h) - f(x)$

By Taylor's Series expansion, we have

$$f(x+h) = f(x) + \frac{h}{1!}f'(x) + \frac{h^2}{2!}f''(x) + \frac{h^3}{3!}f'''(0) + \dots$$

Define $D \equiv \frac{d}{dx}$

so that $f'(x) = Df, f''(x) = D^2 f, f'''(x) = D^3 f, \dots$

$$\therefore f(x+h) = \left[1 + hD + \frac{h^2D^2}{2!} + \frac{h^3D^3}{3!} + \dots\right] f(x)$$

$$= e^{hD} f(x) \qquad \left(\because e^x = 1 + x + \frac{x^2}{2!} + \dots\right)$$

Now, $\Delta f(x) = f(x+h) - f(x)$

$$\Delta f(x) = e^{hD} f(x) - f(x)$$

$$\Rightarrow \Delta f(x) = (e^{hD} - 1) f(x)$$

$$\therefore \Delta \equiv e^{hD} - 1$$

$$\Rightarrow e^{hD} \equiv 1 + \Delta$$

Taking Log on both sides, we get $hD \equiv \log(1+\Delta)$

$$\Rightarrow hD \equiv \Delta - \frac{\Delta^2}{2} + \frac{\Delta^3}{3} - \frac{\Delta^4}{4} + \dots \qquad \Rightarrow D \equiv \frac{1}{h}\left(\Delta - \frac{\Delta^2}{2} + \frac{\Delta^3}{3} - \frac{\Delta^4}{4} + \dots\right)$$

$$\Rightarrow Dy_i \equiv \frac{1}{h}\left(\Delta - \frac{\Delta^2}{2} + \frac{\Delta^3}{3} - \frac{\Delta^4}{4} + \dots\right) y_i$$

$$\Rightarrow \left(\frac{dy}{dx}\right)_{y=y_i} = \frac{1}{h}\left(\Delta y_i - \frac{\Delta^2}{2} y_i + \frac{\Delta^3}{3} y_i - \frac{\Delta^4}{4} y_i + \dots\right)$$

To find Second Derivative

We have $hD \equiv \Delta - \frac{\Delta^2}{2} + \frac{\Delta^3}{3} - \frac{\Delta^4}{4} + \dots$

Squaring on both sides, we get $(hD)^2 \equiv \left(\Delta - \frac{\Delta^2}{2} + \frac{\Delta^3}{3} - \frac{\Delta^4}{4} + \ \dots\right)^2$

$$\Rightarrow h^2D^2 \equiv \left(\Delta - \frac{\Delta^2}{2} + \frac{\Delta^3}{3} + \ \dots\right)^2$$

$$\equiv \left(\Delta^2 + \frac{\Delta^4}{4} + \frac{\Delta^6}{9} - \Delta^3 - \frac{\Delta^5}{3} + \frac{2}{3}\Delta^4 + \cdots\right) (\because\ (a-b+c)^2 = a^2 + b^2 + c^2 - 2ab - 2bc + 2ca)$$

$$\equiv \left(\Delta^2 - \Delta^3 + \frac{11}{12}\Delta^4 + \ \dots\right)$$

$$\Rightarrow D^2 \equiv \frac{1}{h^2}\left(\Delta^2 - \Delta^3 + \frac{11}{12}\Delta^4 + \ \dots\right)$$

$$\Rightarrow \ \left(\frac{d^2y}{dx^2}\right)_{x=x_i} \equiv \frac{1}{h^2}\left(\Delta^2 y_i - \Delta^3 y_i + \frac{11}{12}\Delta^4 y_i + \ \dots\right)$$

To find Third Derivative

We have $hD \equiv \Delta - \frac{\Delta^2}{2} + \frac{\Delta^3}{3} - \frac{\Delta^4}{4} + \ \dots$

Cubing on both sides, we get $(hD)^3 \equiv \left(\Delta - \frac{\Delta^2}{2} + \frac{\Delta^3}{3} - \frac{\Delta^4}{4} + \ \dots\right)^3$

$$\Rightarrow h^3D^3 \equiv \left(\Delta - \frac{\Delta^2}{2} + \ \dots\right)^3$$

$$\Rightarrow h^3D^3 \equiv \left(\Delta^3 - \frac{\Delta^6}{8} - \frac{3}{2}\Delta^4 + \frac{3}{4}\Delta^5 + \ \dots\right) \ (\because (a-b)^3 = a^3 - b^3 - 3a^2b + 3ab^2)$$

$$\Rightarrow D^3 \equiv \frac{1}{h^3}\left(\Delta^3 - \frac{3}{2}\Delta^4 + \ \dots\right)$$

$$\Rightarrow \left(\frac{d^3y}{dx^3}\right)_{x=x_i} \equiv \frac{1}{h^3}\left(\Delta^3 y_i - \frac{3}{2}\Delta^4 y_i + \ \dots\right)$$

Differentiation using Backward differences

We know that $\nabla f(x) = f(x) - f(x-h)$

By Taylor's Series expansion, we have

$$f(x-h) = f(x) - \frac{h}{1!}f'(x) + \frac{h^2}{2!}f''(x) - \frac{h^3}{3!}f'''(0) + \ \dots$$

Define $D \equiv \frac{d}{dx}$

so that $f'(x) = Df, f''(x) = D^2 f\ , f'''(x) = D^3 f, \dots$

$$\therefore f(x-h) = \left[1 - hD + \frac{h^2D^2}{2!} - \frac{h^3D^3}{3!} + \ \dots\right] f(x)$$

$$= e^{-hD} f(x) \quad \left(\because\ e^{-x} = 1 - x + \frac{x^2}{2!} - \ \dots\right)$$

Now, $\nabla f(x) = f(x) - f(x-h)$

$$\nabla f(x) = f(x) - e^{-hD} f(x)$$

$$\Rightarrow \ \nabla f(x) = (1 - e^{-hD}) f(x)$$

$$\therefore \ \nabla \equiv 1 - e^{-hD}$$

$$\Longrightarrow \ e^{-hD} \equiv 1 - \nabla$$

Taking Log on both sides, we get $-hD \equiv \log(1-\nabla)$

$$\Longrightarrow -hD \equiv -\nabla - \frac{\nabla^2}{2} - \frac{\nabla^3}{3} - \frac{\nabla^4}{4} + \ \dots \qquad \Longrightarrow D \equiv \frac{1}{h}\left(\nabla + \frac{\nabla^2}{2} + \frac{\nabla^3}{3} + \frac{\nabla^4}{4} + \ \dots\right)$$

$$\Longrightarrow Dy_i \equiv \frac{1}{h}\left(\nabla + \frac{\nabla^2}{2} + \frac{\nabla^3}{3} + \frac{\nabla^4}{4} + \ \dots\right) y_i$$

$$\Longrightarrow \ \left(\frac{dy}{dx}\right)_{y=y_i} = \frac{1}{h}\left(\nabla y_i + \frac{\nabla^2}{2} y_i + \frac{\nabla^3}{3} y_i + \frac{\nabla^4}{4} y_i + \ \dots\right)$$

To find Second Derivative

We have $hD \equiv \nabla + \frac{\nabla^2}{2} + \frac{\nabla^3}{3} + \frac{\nabla^4}{4} + \ \dots$

Squaring on both sides, we get $(hD)^2 \equiv \left(\nabla + \frac{\nabla^2}{2} + \frac{\nabla^3}{3} + \frac{\nabla^4}{4} + \ \dots\right)^2$

$$\Longrightarrow h^2D^2 \equiv \left(\nabla + \frac{\nabla^2}{2} + \frac{\nabla^3}{3} + \ \dots\right)^2$$

$$\equiv \left(\nabla^2 + \frac{\nabla^4}{4} + \frac{\nabla^6}{9} + \nabla^3 + \frac{\nabla^5}{3} + \frac{2}{3}\nabla^4 + \cdots\right) (\because \ (a+b+c)^2 = a^2 + b^2 + c^2 + 2ab + 2bc + 2ca)$$

$$\equiv \left(\nabla^2 + \nabla^3 + \frac{11}{12}\nabla^4 + \ \dots\right)$$

$$\Longrightarrow D^2 \equiv \frac{1}{h^2}\left(\nabla^2 + \nabla^3 + \frac{11}{12}\nabla^4 + \ \dots\right)$$

$$\Longrightarrow \ \left(\frac{d^2y}{dx^2}\right)_{x=x_i} \equiv \frac{1}{h^2}\left(\nabla^2 y_i + \nabla^3 y_i + \frac{11}{12}\nabla^4 y_i + \ \dots\right)$$

To find Third Derivative

We have $hD \equiv \nabla + \frac{\nabla^2}{2} + \frac{\nabla^3}{3} + \frac{\nabla^4}{4} + \ \dots$

Cubing on both sides, we get $(hD)^3 \equiv \left(\nabla + \frac{\nabla^2}{2} + \frac{\nabla^3}{3} + \frac{\nabla^4}{4} + \ \dots\right)^3$

$$\Longrightarrow h^3D^3 \equiv \left(\nabla + \frac{\nabla^2}{2} + \ \dots\right)^3$$

$$\Longrightarrow h^3D^3 \equiv \left(\nabla^3 + \frac{\nabla^6}{8} + \frac{3}{2}\nabla^4 + \frac{3}{4}\nabla^5 + \ \dots\right) \ (\because (a+b)^3 = a^3 + b^3 + 3a^2b + 3ab^2)$$

$$\Longrightarrow D^3 \equiv \frac{1}{h^3}\left(\nabla^3 + \frac{3}{2}\nabla^4 + \ \dots\right)$$

$$\Longrightarrow \left(\frac{d^3y}{dx^3}\right)_{x=x_i} \equiv \frac{1}{h^3}\left(\nabla^3 y_i + \frac{3}{2}\nabla^4 y_i + \ \dots\right)$$

Differentiation using Central differences

We know that the Stirling's Formula is given by

$$y = y_0 + \frac{p}{2}(\Delta y_0 + \Delta y_{-1}) + \frac{p^2}{2}\Delta^2 y_{-1} + \frac{(p^3-p)}{12}(\Delta^3 y_{-1} + \Delta^3 y_{-2}) + \frac{(p^4-p^2)}{24}\Delta^4 y_{-2} + \ \dots$$

Where $p = \frac{x-x_0}{h}$

Now, Differentiating w.r.t. x, we get $\frac{dy}{dx} = \frac{dy}{dp} \cdot \frac{dp}{dx}$

$\frac{dy}{dx} = \frac{1}{h} \cdot \frac{dy}{dp}$ $\qquad \left(\because \frac{dp}{dx} = \frac{1}{h}\right)$

$$\Rightarrow \frac{dy}{dx} = \frac{1}{h}\left(\frac{1}{2}(\Delta y_0 + \Delta y_{-1}) + p\Delta^2 y_{-1} + \frac{(3p^2-1)}{12}(\Delta^3 y_{-1} + \Delta^3 y_{-2}) + \frac{(4p^3-2p)}{24}\Delta^4 y_{-2} + \ \dots\right)$$

At $x = x_0 \Rightarrow p = 0$

$$\Rightarrow \left(\frac{dy}{dx}\right)_{x=x_0} = \frac{1}{h}\left(\frac{1}{2}(\Delta y_0 + \Delta y_{-1}) - \frac{1}{12}(\Delta^3 y_{-1} + \Delta^3 y_{-2}) + \ \dots\right)$$

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

$$\left(\frac{d^3y}{dx^3}\right)_{x=x_0} = \frac{1}{h^3}\left(\frac{1}{2}(\Delta^3 y_{-1} + \Delta^3 y_{-2}) + \ \dots\right)$$

When we have to use these formulae?

When we are asked to find $\frac{dy}{dx}$ at the point $x = x_i$, the problem analyzing should be as follows:

If the point $x = x_i$ is nearer to the starting arguments of the given table, then use Forward difference formulas for differentiation

If the point $x = x_i$ is nearer to the ending arguments of the given table, then use Backward difference formulas for differentiation

If the point $x = x_i$ is nearer to the Middle arguments of the given table, then use Central difference formulas for differentiation.

Numerical Integration

We know that a definite integral of the form $\int_a^b f(x)dx$ represents the area under the curve $y = f(x)$, enclosed between the limits $x = a$ and $x = b$.

Let $I = \int_a^b f(x)dx$. Here the value of I is a Numerical value.

Aim: To find the approximation to the Numerical value of I. The process of finding the approximation to the definite Integral is known as Numerical Integration.

Let $x_0, x_1, x_2, \dots, x_n$ be given set of observations, and let $y_0, y_1, y_2, \dots, y_n$ be the corresponding values for the curve $y = f(x)$.

$$I \cong h\int_0^n \left[f_0 + s\frac{\Delta f_0}{1!} + s(s-1)\frac{\Delta^2 f_0}{2!} + \ \dots + s(s-1)(s-2)\dots(s-[n-1])\frac{\Delta^n f_0}{n!}\right] ds$$

This formulae is also known as Newton Cotes closed type Formulae.

- If $n = 1$, the formula is known as Trapezoidal Rule
- If $n = 2$, the formula is known as Simpson's $\frac{1}{3}rd$ Rule

- If $n = 3$, the formula is known as Simpson's $\frac{3}{8}th$ Rule

Trapezoidal Rule

$$I \cong \frac{h}{2}[(y_0 + y_n) + 2(y_1 + y_2 + y_3 + \ ... + y_{n-1})]$$

i.e. $I \cong \frac{h}{2}[(First\ term + Last\ term) + 2(Sum\ of\ remaining\ terms)]$

Here n is number of Intervals, and $h = \frac{b-a}{n}$

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

$$I \cong \frac{h}{2}[(y_0 + y_{2n}) + 4(y_1 + y_3 + \ ... + y_{2n-1}) + 2(y_2 + y_4 + \cdots + y_{2n-2})]$$

i.e. $I \cong \frac{h}{2}[(First\ term + Last\ term) + 4(Sum\ of\ odd\ terms) + 2(sum\ of\ even\ terms)]$

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

$$I \cong \frac{h}{2}[(y_0 + y_{3n}) + 3(y_1 + y_2 + y_4 + y_6 + \ ... + y_{3n-1}) + 2(y_3 + y_6 + \cdots + y_{3n-3})]$$

i.e. $I \cong \frac{h}{2}[(First\ term + Last\ term) + 3(Sum\ of\ terms\ which\ are\ not\ multiples\ of\ 3) +$
2(sum of terms which are multiples of 3)

- If Even number of Intervals are there, it is preferred to use Simpson's $\frac{1}{3}rd$ Rule (Or) Trapezoidal Rule.
- If Number of Intervals is multiple of 3, then use Simpson's $\frac{3}{8}th$ Rule (Or) Trapezoidal Rule.
- If Odd number of Intervals are there, and which is not multiple of 3, then use Trapezoidal Rule. Ex: 5, 7 etc.
- For any number of Intervals, the default Rule we can use is Trapezoidal.

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