This question paper contains 4 printed pages.]

3407 *Your Roll No. .....*

M. Tech. / II Sem. A

NANO SCIENCE AND NANO TECHNOLOGY

Paper NSNT–202 : Computational Methods

Time : 3 Hours *Maximum Marks : 38*

(Write your Roll No. on the top immediately on receipt of this question paper.)

*Answer any **four** questions.*
All questions carry equal marks.

1. (a) Using Newton's forward difference formula for n=2 obtain Simpson's $\frac{1}{3}$ formula for evaluation of a definite integral. Work out the errors involved in this method. 5½

(b) Use four point Gauss-Legendre formula to evaluate the integral $\int_0^1 \frac{1}{1+x^2}\,dx$

Abscissae and weights are

$\pm u_i = 0.33998 : w_i = 0.65215$

$\pm u_i = 0.86114 : w_i = 0.34785$ 4

[P.T.O.

2. (a) Obtain the expressions for the best value of the slope and intercept and their standard errors by the method of points in pairs using least square method. Write these expressions in the form of summations containing only variable x_i and y_i. 5½

(b) A group of students measured resistance of a wire and obtain the following values in ohms : 5.321, 5.311, 5.295; 5.305; 5.292; 5.285; 5.301; 5.293; 5.287 and 5.310. From residuals and (residuals)^2, estimate σ by the standard method. Give the best value of resistance with its error (σ_m) for the group. 4

3. (a) Establish Newton's forward difference interpolation formula and the remainder terms (error in the formula) in terms of appropriate derivatives. From the following data of values of x and $f(x)$ determine $f(6.36)$: data for x and $f(x)$ is : (6.1 : 226.981); (6.2 : 238.328); (6.3:250.047); (6.4 : 262.144); (6.5 : 274.625); (6.6 : 287.496); (6.7 : 300.763) 5½

(b) Define the operators Δ, ∇, δ, E and μ and show

(i) $\Delta - \nabla = \delta^2$

(ii) $1 + \Delta = (E - 1)\nabla^{-1}$

(iii) $\mu E = E, 4$ 4

4. (a) Discuss the finite difference method in a two point linear boundary value problem in an ordinary differential equation and estimate the error involved in this method.

A boundary-value problem is defined by

$$\frac{d^2y}{dx^2} + y + 1 = 0 \quad 0 \le x \le 1$$

where $y(0) = 0$ and $y(1) = 0$

taking $h = 0.25$, use the finite-difference method to determine the value of $y(0.25)$ and $y(0.5)$. 6½

(b) Use second order Runge-Kutta formula to find $y(0.3)$ for a differential equation $\frac{dy}{dx} = x + y$; $y(0) = 1$: take $h = 0.1$ 3

5. (a) Consider a system of n linear equations with n unknown and use Gauss-Elimination method to solve it by converting into equivalent upper triangular system.

Use this method to solve

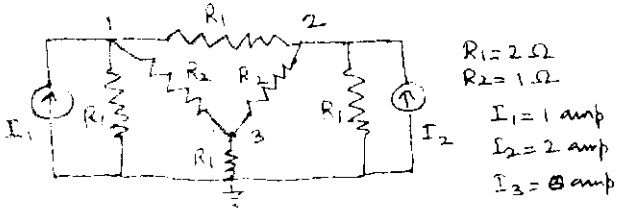
$2x + y + z + t = 12$

$3x + 2y + 3z - t = 16$

$x + 4y + 9z + 3t = 22$

$x + y + 3z + 4t = 21$ 5½

(b) Write the admittance and current matrix of the following circuit and find the voltage vector using matrix operations. 4



6. Attempt any **two** of the following :

(i) Obtain the electron-density equation for a crystal in terms of scattering amplitude and position of the atoms in a crystal using Fourier transforms. 4¾

(ii) Use Newton-Raphson method to obtain a root, correct to three decimal places of the equation $e^x = \cot x$. 4¾

(iii) Discuss the iteration method of root-finding in detail and how acceleration of convergence can be improved using Aitken's Δ^2–process. 4¾