PHL 800: Numerical and Computational Methods in Research

(IInd Semester, 2006-2007)

MAJOR TEST

Duration: 2 hours **Max. Marks: 50**

Q.1-6 carry 5 marks each and Q.7-10 carry 10 marks each.
Attempt questions for a total of 50 marks.

1. The equation: $x^3 + 3x^2 + 48 = 0$ has one real root α and two complex roots $\beta \pm i\gamma$. Determine the values of α using the Newton-Raphson method and then find the two complex roots by using the relations obtained using the theory of equations involving the sum of the roots and the products of the roots. 5

2. Consider the following differential equation 5

$$\frac{d^2y}{dx^2} + \pi^2 y = 0 \quad \text{with} \quad \left.\frac{dy}{dx}\right|_{x=0} = \pi \quad \text{and} \quad y(0) = 0,$$

the solution of which is $y(x) = \sin(\pi x)$. Use the fourth-order Runge-Kutta method to obtain the value of $\sin(\pi/4)$ using $h = 0.125$.

3. The exponential integral function $y = E_1(x)$ satisfies the differential equation: 5

$$\frac{dy}{dx} = -\frac{e^{-x}}{x}.$$

Some of the values of the function are given below. Use Milne's method to obtain $E_1(1.2)$.

x	0.7	0.8	0.9	1.0	1.1
$E_1(x)$	0.374	0.311	0.260	0.219	0.186

4. Use Simpson's rule to evaluate the following integral using the data given in Q.2: 5

$$\int_{0.7}^{1.1} E_1(x)\,dx$$

5. Consider a set of 1000 random number pairs (x_i, y_i) each of which lies in the range of (0,1). Write the main steps to generate 500 random points in a circular region defined by $x^2 + y^2 = 1$. 5

6. Consider the matrices 3+2

$$\mathbf{A} = \begin{pmatrix} 2 & 1 & 0 \\ 1 & 2 & 0 \\ 0 & 0 & 2 \end{pmatrix}; \qquad \mathbf{X} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

(a) Use the partition method to obtain the inverse of this matrix **A**.
(b) The eigenvalues of the matrix A are 1,2,3. If the power method is used to obtain the largest eigenvalue of **A** using the column vector **X** as the starting vector, we get an eigenvalue as 2. Explain the reason.

7. Discuss the principle of the Galerkin method, ***OR***, the collocation method, and give the procedure for obtaining the matrix eigenvalue equation for the time-independent Schrödinger equation: 10

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V(x)\psi(x) = E\psi(x)$$

8. In an experiment following set of data is obtained 10

t	0.0	0.5	1.0	2.0
$f(t)$	0.00	0.57	1.46	5.05

These are supposed to follow the functional behavior as $f(t) = ae^{bt} + c$ and it is known that $b \approx 1$.

(i) Obtain a & c using the least square method assuming $b = 1$.

(ii) Use these values of a & c, to obtain a better value of b, gain using the least square method.

9. (a) Starting with 4+6

$$\frac{1}{2h}\int_0^{2h} M\,dx = \left.\frac{d^2y}{dx^2}\right|_{x=h}$$

obtain the procedure for cubic spline fitting. Interpret the above equation geometrically.

(b) Consider the following data

x	0	1	2	3
$f(x)$	1	5	75	250

and assume $M(0) = 0$ and $M(3) = 0$. Obtain the cubic spline approximation in each interval.

10. (a) Show that an interpolating polynomial obtain for a given set of data is unique irrespective of the method of obtaining it. 4+6

(b) Find the polynomial of degree 2 or less, such that $f(0) = 1, f(1) = 3$ and $f(3) = 55$ using the Lagrange interpolation method.

Formulae:

A. Runge-Kutta Method (4th Order)

$$\frac{dy}{dx} = f[x, y]$$
$$y(x+h) = y(x) + \tfrac{1}{6}(K_1 + 2K_2 + 2K_3 + K_4)$$
$$K_1 = hf[x, y(x)]$$
$$K_2 = hf[x + \tfrac{1}{2}h, y(x) + \tfrac{1}{2}K_1]$$
$$K_3 = hf[x + \tfrac{1}{2}h, y(x) + \tfrac{1}{2}K_2]$$
$$K_4 = hf[x + h, y(x) + K_3]$$

B. Cubic Spline Fitting

$$M_{i-1} + 4M_i + M_{i+1} = \frac{6}{h}(y_{i+1} - 2y_i + y_{i-1})$$

C. Milne's method: P: $y_{n+1} = y_{n-3} + (4h/3)(2y'_n - y'_{n-1} + 2y'_{n-2})$

C: $y_{n+1} = y_{n-1} + (h/3)(y'_{n-1} + 4y'_n + y'_{n+1})$

D. Simpson's Rule

$$\int_0^{2h} f(x)dx = (h/3)[f(0) + 4f(h) + f(2h)]$$