Registration No. $\square$

Total number of pages : 04
B.Tech.

PCE6I101
$6^{\text {th }}$ Semester Regular Examination 2017-18
NUMERICAL METHODS \& MATLAB
BRANCH : CHEM
Time : 3 Hours
Max Marks $: 100$
Q.CODE $:$ C141
Answer Part-A which is compulsory and any four from Part-B.
The figures in the right-hand margin indicate marks.
Assume suitable notations and any missing data wherever necessary.
Answer all parts of a question at a place.

## Part-A (Answer all the questions)

Q1.
Answer the following questions:
(a)
$X n)$.
i. Interpolation
ii. Extrapolation
iii. Iterative
iv. Polynomial equation
(b) Lagrange's interpolation formula is used to compute the values for $\qquad$ intervals.
i. Equal
ii. Unequal
iii. Open
iv. Closed
(c) Romberg's method is also known as $\qquad$ .
i. Trapezoidal rule
ii. Simpson's (1/3)rd Rule
iii. Simpson's (3/8)th Rule
iv. Rombergs Integration
(d) In Simpson's 1/3rd rule the number of intervals must be $\qquad$ .
i. A multiple of 3
ii. A multiple of 6
iii. Odd
iv. Even
(e)

The Eigenvalues of $\left[\begin{array}{ccc}5 & 6 & 17 \\ 0 & -19 & 23 \\ 0 & 0 & 37\end{array}\right]$ are
i. $37,5,-19$
ii. $-37,-5,19$
iii. $7,-3,2$
iv. $37,-5,3$
(f) The Eigen values of a $4 \times 4$ matrix $[A]$ are given as $2,-3,13$, and 7 . The $\operatorname{det}(A)$ is
$\qquad$ 546
ii. 19
iii. 25
iv. Cannot be determined
(g) $y(x+h)=y(x)+h f(x, y)$ is referred as $\qquad$ method.
i. Euler
ii. Modified Euler
iii. Taylor's Series
iv. Runge-Kutta
(h) The power method for approximating Eigen value is $\qquad$ method.
i. Iterative
ii. Point-wise
iii. Direct
iv. Indirect
(i)

The partial differential equation $5 \frac{\partial^{2} z}{\partial x^{2}}+6 \frac{\partial^{2} z}{\partial y^{2}}=x y$ is classified as
i. Elliptic
ii. Parabolic
iii. Hyperbolic
iv. None of these
(j) A partial differential equation requires
i. Exactly one independent variable
ii. Two or more independent variables
iii. More than one dependent variable
iv. Equal number of dependent and independent variables

Q2. Answer the following questions:
(a) If $\mathrm{Y}\left(\mathrm{X}_{\mathrm{i}}\right)=\mathrm{Y}_{\mathrm{i}}, \mathrm{i}=0,1,2, \ldots$, n write down the formula for the cubic spline polynomial $Y(X)$ valid in $X_{i-1} \leq X \leq X_{i}$.
(b) What is interpolation? What is the difference between interpolation and extrapolation?
(c) State Forward divided difference formula for finding $\mathrm{F}^{\prime}(\mathrm{x})$ and $\mathrm{f}^{\prime \prime}(\mathrm{x})$.
(d) The table given below reveals the velocity $v$ of a body during the time $t$ specified. Find its acceleration at $\mathrm{t}=1.1$.

| T (in sec) | 1.0 | 1.1 | 1.2 | 1.3 | 1.4 |
| :--- | :--- | :--- | :--- | :--- | :--- |
| V (in $\mathrm{m} / \mathrm{s}$ ) | 43.1 | 47.7 | 52.1 | 56.4 | 60.8 |

(e) Define Discrete Fourier Transform and algebraic form of FFT.
(f)

Find a QR factorization of a matrix $\left[\begin{array}{ll}3 & 7 \\ 4 & 4\end{array}\right]$.
(g) What is the need of numerical solution for differential equations?
(h) "Multistep methods are not self-starting". Justify.
(i) State the condition of the equation $\mathrm{Au}_{\mathrm{xx}}+\mathrm{Bu}_{\mathrm{yy}}+\mathrm{Cu}_{\mathrm{yy}}+\mathrm{Du}_{\mathrm{x}}+\mathrm{Eu}_{\mathrm{y}}+\mathrm{Fu}=\mathrm{G}$ where A, B, C, D, E, F, G are functions of $x$ and $y$ to be (i) elliptic (ii) parabolic (iii) hyperbolic.
(j) Write down Adam-Bashforth predictor formula.

## Part - B (Answer any four questions)

Q3. (a) The following table gives some relationship between steam pressure and temperature. Find the pressure at temperature 372 using piecewise linear interpolation.

| $\mathbf{T}(\mathbf{K})$ | 361 | 367 | 378 | 387 | 399 |
| :--- | :--- | :--- | :--- | :--- | :--- |
| $\mathbf{P ( k P a})$ | 154.9 | 167.9 | 191.0 | 212.5 | 244.2 |

(b) Find the second derivative at $\mathrm{x}=4$, using the following data:

| $x$ | 0 | 2 | 4 | 6 |
| :--- | :--- | :--- | :--- | :--- |
| $y$ | 2 | 5 | 8 | 14 |

(c) Find the values of $f^{\prime \prime}(0.2), f^{\prime \prime}(0.6), f^{\prime}(1.0)$ from the following data using appropriate initial values based on finite difference and Richardson's extrapolation method.

| $\mathbf{x}$ | 0.2 | 0.4 | 0.6 | 0.8 | 1.0 |
| :--- | :--- | :--- | :--- | :--- | :--- |
| $\mathbf{F}(\mathbf{x})$ | 0.12 | 0.49 | 1.12 | 2.02 | 3.20 |

Q4. (a)
Compute $\mathrm{I}=\int_{0}^{\frac{\pi}{3}} \tan x d x$, using Simpson's rule with $\mathrm{h}=\pi / 6, \pi / 12, \pi / 24$ and then by Romberg's method.
(b) Using Hermite's interpolation formula estimate the value of $\operatorname{In} 3.2$ from the following data

| $\mathbf{x}$ | $\mathbf{F}(\mathbf{x})=\mathbf{\operatorname { l n } \mathbf { x }}$ | $\mathbf{F}^{\prime}(\mathbf{x})=\mathbf{1 / x}$ |
| :--- | :--- | :--- |
| 3.0 | 1.09861 | 0.33333 |
| 3.5 | 1.25276 | 0.28571 |
| 4.0 | 1.38629 | 0.25 |

Q5. (a) Find the dominant Eigen value of the following matrix by power method and compare with Rayleigh's quotient method.

$$
A=\left[\begin{array}{ccc}
2 & -1 & 0 \\
-1 & 2 & -1 \\
0 & -1 & 2
\end{array}\right]
$$

(b) The differential equation $\frac{d y}{d x}=y-x^{2}$ satisfied by $y(0)=1, y(0.2)=1.1218$, $y(0.4)=1.4282, y(0.6)=1.7379$. Compute $y(0.8)$ by Milne's predictor-corrector method.

Q6. (a) Find the QR factorization of the matrix $\left[\begin{array}{lll}1 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 1\end{array}\right]$ using Gram Schmidt process.
(b) Compute 4-point DFT of the following sequence using DIT and DIF algorithms.

$$
X(n)=\{0,1,2,3\}
$$

Q7. Find the numerically smallest Eigen value of the matrix $A$ by finding $A^{-1}$ and without finding $A^{-1}$ given that one of the Eigen values of $A$ is -20 .

$$
A=\left[\begin{array}{ccc}
-15 & 4 & 3  \tag{15}\\
10 & -12 & 6 \\
20 & -4 & 2
\end{array}\right]
$$

Q8. Solve $25 u_{x x}-u_{t t}=0$ for $u$ with the boundary conditions $u(0, t)=0, u(5, t)=0$ and the initial conditions $u_{t}(x, 0)=0$ and $u(x, 0)=2 x$ for $0 \leq x \leq 2.5 u(x, 0)=10-2 x$ for $2.5 \leq x \leq 5$, taking $\mathrm{h}=1$.(for four time steps)

Q9. (a) Given $\frac{\partial^{2} f}{\partial x^{2}}=\frac{\partial f}{\partial t}$,
Subject to $f(0, t)=f(5, t)=0, f(x, 0)=x^{2}\left(25-x^{2}\right)$.
Find f in the range taking $\mathrm{h}=1$ and up to 5 seconds.
(b) Solve $\nabla^{2} u=-10\left(x^{2}+y^{2}+10\right)$ over the square mesh with sides $x=0, y=0, x=3, y=3$ with $u=0$ on the boundary and mesh length is 1 unit.

