UNIVERSITY OF CALCUTTA

Notification No. CSR/12/2025

It is notified for information of all concerned that in terms of the provisions of Section 54 of the Calcutta University Act, 1979, (as amended), and, in the exercise of her powers under 9(6) of the said Act, the Vice-Chancellor has, by an order dated 18.02.2025 approved the "Model Questions" of semester-3 (Paper: CHEM-H-SEC3-3-Th) of 4-Year Honours and Honours with Research, Courses of Studies in Chemistry, under CCF.

The new CSR shall take immediate effect.

25/02/2025

SENATE HOUSE

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25.02.2025

Prof.(Dr.) Debasis Das

Registrar

REGISTRAR
UNIVERSITY OF CALCUTTA

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BSc. Chemistry Major (Under CCF,2022)

Model Questions

Paper: CHEM-H-SEC3-3-Th

(Introduction to Numerical Methods for Chemists)

1. a) What do you mean by fixed point representation? Why is it inconvenient in most cases?
   b) What is the IEEE754 single precision floating point representation of (i) -0.8125, and (ii) 9.27?
   c) Express the following decimal number in the binary form: (i) 22.625, (ii) 6.0, (ii) -10.125
   d) What is NAN in IEEE floating point standard?

2. a) Graphically explain Newton-Raphson iterative method.
   b) Deduce Newton-Raphson equation using Taylor series approximation.
   c) Find a root of the equation x sin x + cos x =0 using Newton-Raphson method. Taking initial guess as $x_0 = \pi$.
   d) Find a real root of the equation $x = e^{-x}$. considering initial guess as $x_0 = 1$.
   e) Consider the chemical reaction described by the equation:
   $CH_4(g) + H_2O(g) = CO(g) + 3H_2(g)$
   At 300K. If 1.00 bar of CH_4 (g) and H_2O (g) are introduced into a reaction vessel, the equilibrium constant $K_p = 26$.
   Solve using Newton-Raphson method up to four significant figures to obtain the partial pressure of CO at equilibrium. Consider the initial guess of P_{CO} as 0.5.

3. a) What is the difference between interpolation and extrapolation?
   b) Consider the data values (x_0, f_0), (x_1,f_1),(x_2,f_2), ……..(x_n,f_n) with arbitrarily spaced x_i. Obtain Lagrange polynomial for the above set of data.
   c) Consider the following data values:

x	1	2	3	4
f(x)	1	8	27	64

   Find f (2.5) using Lagrange interpolation with a quadratic interpolation polynomial. Repeat the calculation using a cubic interpolating polynomial.

4. a) Determine the constants ‘a’ and ‘b’ by the method of least squares such that $y=a.e^{bx}$ fits the following set of data:

x	2	4	6	8	10
y	4.077	11.084	30.128	81.897	222.62

b) Estimate the value of 'λ' and 'c' by performing least square fit of the equation $PV^{\lambda} = c$ to the given data:

P(atm)	1.13	2.70	5.34	7.86	13.29
V(L)	0,82	0.49	0.33	0.25	0.16

c) What do you mean by 'residual sum of squares' (SSE) and 'total sum of squares'(SST). Express 'Coefficient of determination' (r^2) using SSE and SST.

d) What is Linear Correlation coefficient (r)? What are the properties of 'r'?

5. a) Obtain first order forward difference formula, backward difference formula and central difference formula using Taylor series approximation. Also obtain using graphical representation.

   b) The concentration of reactant A is monitored over time during a reaction. The following data is recorded:

Time t(s)	0	10	20	30	40	50
Concentration [A](mol/L)	1	0.82	0.68	0.55	0.45	0.37

   Use forward, backward and central difference formula to numerically estimate the reaction rate at t = 20 s.

6. a) What is the Trapezoidal rule? Give a geometrical interpretation of the rule. What is the composite trapezoidal rule?
   b) What is the composite midpoint rule?
   c) Derive Simpson's 1/3rd rule from Lagrange interpolation equation.
   d) Give a graphical explanation of the Simpson's 1/3rd rule.

   e) Evaluate $\int_0^1 1/(1+x)dx$ correct to three decimal places, (h=0.5) using both Trapezoidal and Simpson's 1/3rd rule.

7. a) Explain the forward Euler and the backward Euler method.
   b) Use the forward Euler method to solve the initial value problem $y'(x) = xy(x)$, $y(0)=2$ between $0 \leq x \leq 1$. [consider h=0.1]
   c) Solve the differential equation
   $dy/dx + xy = 0$, $y(0) = 1$, between $0 \leq x \leq 0.25$ using the forward Euler method [consider h=0.05]
   c) Graphically explain the second order Runge -Kutta method.
   d)What is Runge-Kutta fourth order method.
   e) Apply Runge-Kutta fourth order method to find an approximate value of y when x = 0.2, given that $dy/dx = x + y$ and $y=1$ when $x=0$.
   f) Apply Runge-Kutta fourth order method to find an approximate value of y when x = 0.2, in steps of 0.1 if $dy/dx = x + y^2$, when x = 0.

8. a) Write down the general expression for the Fourier series. Express Fourier coefficients by the Euler formulas. Deduce all three Euler formulas.
   b) Express Fourier series in terms of any arbitrary period and hence obtain the corresponding Euler formulas.
   c) What are the Fourier Sine and Cosine series?

   d) Obtain the Fourier cosine series for the following function:

$$f(x) = \begin{cases} 0 & \text{if } -2 < x < -1 \\ k & \text{if } -1 < x < 1 \\ 0 & \text{if } 1 < x < 2 \end{cases} \qquad p=2L=4,\ L=2$$

   e) Find the Fourier cosine transform of $\exp(-x^2)$.

   f) Find the Fourier sine transform of e^{-ax}/x.

   g) Find the Fourier cosine transform of

$$f(x) = \begin{cases} x, & \text{for } 0 < x < 1 \\ 2-x, & \text{for } 1 < x < 2 \\ 0, & \text{for } x > 2 \end{cases}$$