

Practice Quiz – 1 of Computational Techniques (Modules 1 to 5)

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Problem 1: Multiple Choice Questions (negative marks for wrong answers)

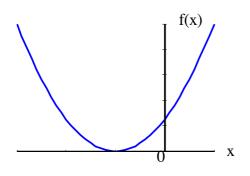
In the following problems, indicate only one correct answer. Each correct answer earns <u>3 points</u>, and wrong answer loses <u>-1 point</u>. There is no negative marking for not attempting the question.

1. Consider the linear equation Ax = b. Let us express A = L + D + U, where L is a lower triangular matrix, D is a diagonal matrix and U is an upper triangular matrix. All diagonal elements of L and U matrices are zero. Using this definition, we can write: Dx = -(L+U)x + b. This yields us:

$$x^{(i+1)} = D^{-1} \left[b - (L+U) x^{(i)} \right]$$

Which of the following iterative methods does the above expression represent?

- a. Jacobi iteration b. Gauss-Seidel
- c. Successive under-relaxation with $\omega = 0.5$ d. None of the above
- 2. Rate of convergence of Newton-Raphson method using analytical Jacobian is:
 - a. Linear b. Quadratic
 - c. Super-linear with power of ~1.618 d. Super-linear with power of ~ $\sqrt{2}$
- 3. Which of the following methods is <u>least suitable</u> for the following function:



a. Reguli Falsi

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b. Secant
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c. Fixed Point Iteration

- d. Newton-Raphson
- 4. Which of the statements are <u>false</u> for Thomas Algorithm
 - a. The computational load increases linearly with number of linear equations
 - b. It can be used even if some of the off-diagonal elements are zero
 - c. Partial pivoting may be required for stability
 - d. Matrix A has to be diagonally dominant to guarantee stability



5. You are given data for variable y at 15 different values of x. Which of the following techniques will result in a curve that is not guaranteed to pass through all the 15 points in X-Y plane?
a. Cubic spline
b. Newton's forward difference
c. Linear regression
d. All of the above

Problem 2: Objective-type questions (No negative marking; no partial credit)

- 1. List all the <u>real roots</u> of the equation $(x^2 + 2)(x + 2)^2(x 3) = 0$
- 2. Some numerical schemes employed to solve n algebraic equations try to minimize errors in all n variables. Hence, the relative error is computed for each of the n variables and stored in a vector <u>ε</u>. The error propagation equation for such a solver is given by <u>ε</u>⁽ⁱ⁺¹⁾ = Γ<u>ε</u>⁽ⁱ⁾. What is the condition on Γ that will ensure that all the errors decrease as the number of iterations increase?
- 3. Consider a quaternary number system, where the base is 4 and the digits can take values 0,1,2,3. A computer uses 6 quaternary digits to store an integer. The first digit is sign digit, and the remaining five digits are used for representing integers. The smallest integer stored by this computer is ______ and the largest integer is ______.
- 4. In the same computer, 16 quaternary digits are used to represent a floating-point number, with one sign digit, 11 digits used for the mantissa and 4 digits for the signed exponent. The machine precision is ______.

Problem 3: Gauss Elimination / LU Decomposition

Consider the linear equation:

$$2x_1 + x_2 + x_3 = 4$$
$$x_1 + 3x_2 + x_3 = 0$$
$$x_1 - x_2 + 3x_3 = 6$$

- 1. Write the above equations in the form Ax = b.
- Compute the upper triangular matrix U using Gauss Elimination. The end result of Gauss Elimination (without back-substitution) is matrix U.
- 3. Compute the lower triangular matrix L. The coefficients used in Gauss Elimination to construct the matrix U form the elements of matrix L. For example, when R_1 is the pivot row, we use $\overline{R_2} = R_2 (1/2)R_1$. Thus, the element $L_{2,1} = 0.5$.
- 4. Find the solution of the above equations using forward and back-substitution.



Problem 4: Newton-Raphson Method (Friction Factor in Turbulent Flow)

The friction factor f depends on the Reynolds number for turbulent flow in a smooth pipe according to the following relationship:

$$\frac{1}{\sqrt{f}} = -0.4 + \sqrt{3}\ln\left(\operatorname{Re}\sqrt{f}\right)$$

Let us define $x = \sqrt{f}$. Now, rearrange the above equation in the standard form: F(x) = 0

With an initial guess of friction factor $f^{\text{initial}} = 0.01$, find the friction factor for Re = 10^5 using four iterations of the Newton-Raphson method. Report the <u>friction factor</u> obtained at the end of each iteration.

Hint-1: Newton Raphson method:

$$x^{(i+1)} = x^{(i)} - \frac{F(x^{(i)})}{F'(x^{(i)})}$$

Hint-2: Do not report x at the end of each iteration, you need to report friction factor, f.

Problem 5: Linear Regression

The rate of an enzymatic reaction is given by the following expression:

$$r = \frac{k[S]}{K_m + [S]}$$

The problem of estimating *k* and *K_m* can be converted to linear regression by inverting the above expression to fit the data to linear equation $y = a_0 + a_1 x$, where: $x = \frac{1}{[S]}$, $y = \frac{1}{r}$

The following data was obtained in the lab:

[<i>S</i>]	0.0975	0.278	0.547	0.632
r	0.0280	0.0531	0.0691	0.0721

- 1. Use linear regression to obtain coefficients for the equation $y = a_0 + a_1 x$
- 2. Hence find the values of k and K_m .

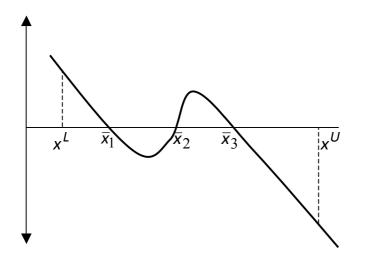
Hint: The least squares values of a_0 and a_1 for linear regression are obtained as a solution of the following equations:

$$a_{0} + a_{1}\left[\sum_{i} x_{i}\right] = \left[\sum_{i} y_{i}\right]$$
$$a_{0}\left[\sum_{i} x_{i}\right] + a_{1}\left[\sum_{i} x_{i}^{2}\right] = \left[\sum_{i} x_{i} y_{i}\right]$$



Problem 6: Descriptive Problem

Two friends Sai and Saanvi are having an argument regarding Bisection method to get the solution for f(x) shown below, where x^L and x^U are two initial guesses (such that <u>all three</u> <u>solutions are bracketed</u> by these guesses). Saanvi tells Sai that for an <u>arbitrary</u> choice of the initial guesses, Bisection method will never yield one of the three solutions to f(x) = 0. Sai disagrees and says that it is possible to get all solutions. Who is correct? Please explain why.



Problem 7: Linear Equations – Gauss-Siedel Method

Consider the following two linear equations to be solved using Gauss-Siedel method:

$$x + 2y = 1$$
$$x - y = 4$$

Use four iterations of the Gauss-Siedel method and report the values of [x, y] at each iteration.

What do you observe? What can you do to make the method converge? Explain.

Hint: *k*th iteration of Gauss Siedel method for N equations is given by:

$$x_i^{(k+1)} = \frac{b_i - \sum_{j=1}^{i-1} a_{ij} x_j^{(k+1)} - \sum_{j=i+1}^{N} a_{ij} x_j^{(k)}}{a_{ii}}$$

Problem 8: Generalization of Héron's Algorithm

Héron's algorithm is arguably the first iterative computational technique known to humans. The square root of 2 can be iteratively calculated using:

$$x^{(i+1)} = \frac{1}{2} \left(x^{(i)} + \frac{2}{x^{(i)}} \right)$$

Use Newton-Raphson method to show that square root of any number *c* can be computed as:

$$x^{(i+1)} = \frac{1}{2} \left(x^{(i)} + \frac{c}{x^{(i)}} \right)$$



Problem 9: Lagrange Interpolation

For the data given in Problem 5, use Lagrange interpolating polynomials to find the rate of reaction for [S] = 0.5. Directly fit the polynomial to r vs. [S] data. Lagrange polynomial is given by: $p(S) = c_1p_1 + c_2p_2 + c_3p_3 + c_4p_4$, where

$$c_i = \frac{r_i}{\prod_{j,j\neq i} (S_i - S_j)}, \quad p_i(S) = \prod_{j,j\neq i} (S - S_j)$$

Hint: $\prod_{j,j\neq 2} (S_2 - S_j)$ means " $(S_2 - S_1)(S_2 - S_3)(S_2 - S_4)$ "

Problem 10: Fixed-Point Iteration

We will use a modified fixed point iteration procedure to find the roots of equation:

$$G(x) \equiv 2 - x + \ln(x) = 0$$

For fixed-point iteration of the form $x^{(i+1)} = g(x^{(i)})$, let us define $g(x) = x + \beta G(x)$.

Find the sufficient condition that fixed-point iteration with the above choice of g(x) converges.

Choose $x^{initial}$ that satisfies the sufficient condition and use fixed-point iteration until the solution reaches desired accuracy of $E_{tol} = 0.001$.

Problem 11: Bisection Method

For the above problem $G(x) \equiv 2 - x + \ln(x) = 0$, estimate how many iterations of bisection method are required if we start with $x^{(L)} = 2$ and $x^{(U)} = 4$, and desire an accuracy of $E_{tol} \equiv |x^{(U)} - x^{(L)}| \le 0.001$.

Epilogue: These are sample problems for practice. The final exam will contain a few multiple-choice questions, a few short/objective-type questions, and approximately 4 regular problems.

Problems worth about 15% of the grade will be repeated in the final exam. This is to motivate students to solve all the problems. (You may have noticed that some problems are repeated in this practice exam from the problem sheet from each module).

We do not expect you to memorize the formulae. Instead, we expect you to understand the numerical techniques, and the procedure to implement and/or derive the formulae.