

S.B.S State University Gurdaspur
Department of Chemical Engineering
Numerical Methods in Chemical Engineering (BTCH-21405)

Assignment No 1
Topic: Measuring Errors

Q1. The derivative of a function $f(x)$ at a particular value of x can be approximately calculated by

$$f'(x) \approx \frac{f(x+h) - f(x)}{h}$$

Of $f'(2)$ for $f(x) = 7e^{0.5x}$ and $h = 0.3$, find

- a) the approximate value of $f'(2)$
- b) the true value of $f'(2)$
- c) the true error for part (a)

Q2. The derivative of a function $f(x)$ at a particular value of x can be approximately calculated by

$$f'(x) \approx \frac{f(x+h) - f(x)}{h}$$

For $f(x) = 7e^{0.5x}$ and $h = 0.3$, find the relative true error at $x = 2$.

Q3. The derivative of a function $f(x)$ at a particular value of x can be approximately calculated by

$$f'(x) \approx \frac{f(x+h) - f(x)}{h}$$

For $f(x) = 7e^{0.5x}$ and at $x = 2$, find the following

- a) $f'(2)$ using $h = 0.3$
- b) $f'(2)$ using $h = 0.15$
- c) Approximate error for the value of $f'(2)$ for part (b)

Q4. If one chooses 6 terms of the Maclaurin series for e^x to calculate $e^{0.7}$, how many significant digits can you trust in the solution? Find your answer without knowing or using the exact answer.

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Assignment No 2
Topic: NONLINEAR EQUATIONS

Q1. You are working for Polymer Industry that makes floats for ABC commodes. The floating ball has a specific gravity of 0.6 and has a radius of 5.5 cm. You are asked to find the depth to which the ball is submerged when floating in water. The equation that gives the depth x to which the ball is submerged under water is given by $x^3 - 0.165x^2 + 3.993 \times 10^{-4} = 0$. Use the bisection method of finding roots of equations to find the depth x to which the ball is submerged under water. Conduct three iterations to estimate the root of the above equation. Find the absolute relative approximate error at the end of each iteration, and the number of significant digits at least correct at the end of each iteration.

Q2. Repeat the problem 1 using Newton-Raphson method of finding roots of equations to find

- a) The depth x to which the ball is submerged under water. Conduct three iterations to estimate the root of the above equation.
- b) The absolute relative approximate error at the end of each iteration, and
- c) The number of significant digits at least correct at the end of each iteration.

Q3. Repeat the problem 1 using secant method of finding roots of equations to find the depth x to which the ball is submerged under water. Conduct three iterations to estimate the root of the above equation. Find the absolute relative approximate error and the number of significant digits at least correct at the end of each iteration.

Q4. Use the false-position method of finding roots of equations to find the depth x to which the ball is submerged under water. Conduct three iterations to estimate the root of the above equation. Find the absolute relative approximate error at the end of each iteration, and the number of significant digits at least correct at the end of third iteration.

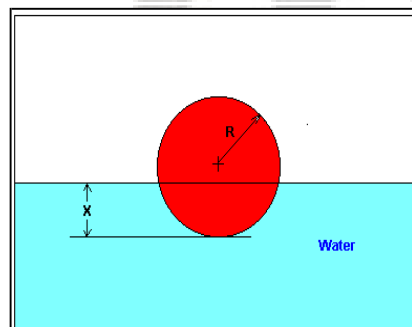


Figure 1 Floating ball problem.

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Assignment No 3
Topic: SIMULTANEOUS LINEAR EQUATIONS

Q1. The upward velocity of a rocket is given at three different times in Table 1.

Table 1 Velocity vs. time data.

Time, t (s)	Velocity, v (m/s)
5	106.8
8	177.2
12	279.2

The velocity data is approximated by a polynomial as

$$v(t) = a_1 t^2 + a_2 t + a_3, \quad 5 \leq t \leq 12$$

The coefficients a_1 , a_2 , and a_3 for the above expression are given by

$$\begin{bmatrix} 25 & 5 & 1 \\ 64 & 8 & 1 \\ 144 & 12 & 1 \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix} = \begin{bmatrix} 106.8 \\ 177.2 \\ 279.2 \end{bmatrix}$$

Find the values of a_1 , a_2 , and a_3 using the Gauss elimination method. Find the velocity at $t = 6, 7.5, 9, 11$ seconds.

Q2. Find the values of a_1 , a_2 , and a_3 using the Gauss-Seidel method. Assume an initial guess of the solution as

$$\begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix} = \begin{bmatrix} 1 \\ 2 \\ 5 \end{bmatrix} \text{ and conduct two iterations.}$$

Q3. Find the eigenvalues and eigenvectors of

$$[A] = \begin{bmatrix} 1.5 & 0 & 1 \\ -0.5 & 0.5 & -0.5 \\ -0.5 & 0 & 0 \end{bmatrix}$$

Q4. Using the LDL^T algorithm, solve the following system for the unknown vector $[x]$.

$$[A][x] = [b] \quad \text{Where} \quad [A] = \begin{bmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 1 \end{bmatrix} \quad [b] = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}$$

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Assignment No 4
Topic: INTERPOLATION

Q1. The upward velocity of a rocket is given as a function of time in Table 1.

Table 1 Velocity as a function of time.

t (s)	0	10	15	20	22.5	30
$v(t)$ (m/s)	0	227.04	362.78	517.35	602.97	901.67

Determine the value of the velocity at $t = 16$ seconds using first order polynomial interpolation by Newton's divided difference polynomial method.

Q2. Using the data in problem 1, determine the value of the velocity at $t = 16$ seconds using second order polynomial interpolation using Newton's divided difference polynomial method.

Q3. Using the data in problem 1, a) Determine the value of the velocity at $t = 16$ seconds with third order polynomial interpolation using Newton's divided difference polynomial method.

b) Using the third order polynomial interpolant for velocity, find the distance covered by the rocket from $t = 11$ s to $t = 16$ s.

c) Using the third order polynomial interpolant for velocity, find the acceleration of the rocket at $t = 16$ s.

Q4. Using the data in problem 1, determine the value of the velocity at $t = 16$ seconds using a first order Lagrange polynomial.

Q5. Using the data in problem 1, (a) Determine the value of the velocity at $t = 16$ seconds with second order polynomial interpolation using Lagrangian polynomial interpolation.

b) Find the absolute relative approximate error for the second order polynomial approximation.

Q6. Using the data in problem 1, (a) Determine the value of the velocity at $t = 16$ seconds using third order Lagrangian polynomial interpolation.

b) Find the absolute relative approximate error for the third order polynomial approximation.

c) Using the third order polynomial interpolant for velocity, find the distance covered by the rocket from $t = 11$ s to $t = 16$ s.

d) Using the third order polynomial interpolant for velocity, find the acceleration of the rocket at $t = 16$ s.

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Assignment No 5
Topic: REGRESSION

Q1. The torque T needed to turn the torsional spring of a mousetrap through an angle, θ is given below, Find the constants k_1 and k_2 of the regression model $T = k_1 + k_2\theta$

Angle, θ Radians	0.698132	0.959931	1.134464	1.570796	1.919862
Torque, T N · m	0.188224	0.209138	0.230052	0.250965	0.313707

Q2. Many patients get concerned when a test involves injection of a radioactive material. For example for scanning a gallbladder, a few drops of Technetium-99m isotope is used. Half of the technetium-99m would be gone in about 6 hours. It, however, takes about 24 hours for the radiation levels to reach what we are exposed to in day-to-day activities. Below is given the relative intensity of radiation as a function of time.

t (hrs)	0	1	3	5	7	9
γ	1.000	0.891	0.708	0.562	0.447	0.355

If the level of the relative intensity of radiation is related to time via an exponential formula $\gamma = Ae^{\lambda t}$, find

- the value of the regression constants A and λ ,
- the half-life of Technium-99m, and
- the radiation intensity after 24 hours.

Q3. The height of a child is measured at different ages as follows.

t (yrs)	0	5.0	8	12	16	18
H (in)	20	36.2	52	60	69.2	70

Estimate the height of the child as an adult of 30 years of age using the growth model,

$H = \frac{a}{1 + be^{-ct}}$, where the constants, a and c are the roots of the simultaneous nonlinear equation system

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Assignment No 6
Topic: INTEGRATION

Q1. The vertical distance covered by a rocket from $t = 8$ to $t = 30$ seconds is given by

$$x = \int_8^{30} \left(2000 \ln \left[\frac{140000}{140000 - 2100t} \right] - 9.8t \right) dt$$

- Use the two-segment trapezoidal rule to find the distance covered from $t = 8$ to $t = 30$ seconds.
- Find the true error, E_t for part (a).
- Find the absolute relative true error for part (a).

Q2. Use 4-segment Simpson's 1/3 rule to approximate the distance covered by a rocket in meters from $t = 8$ s to $t = 30$ s as given by

$$x = \int_8^{30} \left(2000 \ln \left[\frac{140000}{140000 - 2100t} \right] - 9.8t \right) dt$$

- Use four segment Simpson's 1/3rd Rule to estimate x .
- Find the true error, E_t for part (a).
- Find the absolute relative true error, $|\epsilon_t|$ for part (a).

Q3. The vertical distance in meters covered by a rocket from $t = 8$ to $t = 30$ seconds is given by

$$s = \int_8^{30} \left(2000 \ln \left[\frac{140000}{140000 - 2100t} \right] - 9.8t \right) dt$$

Use Simpson 3/8 multiple segments rule with six segments to estimate the vertical distance.

Q4. Compute

$$I = \int_8^{30} \left\{ 2000 \ln \left(\frac{140000}{140000 - 2100t} \right) - 9.8t \right\} dt,$$

Using Simpson 1/3 rule (with $n_1 = 4$), and Simpson 3/8 rule (with $n_2 = 3$).

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Assignment No 7
Topic: ORDINARY DIFFERENTIAL EQUATIONS

Q1. A ball at 1200K is allowed to cool down in air at an ambient temperature of 300K . Assuming heat is lost only due to radiation, the differential equation for the temperature of the ball is given by

$$\frac{d\theta}{dt} = -2.2067 \times 10^{-12} (\theta^4 - 81 \times 10^8), \theta(0) = 1200\text{K}$$

Where θ is in K and t in seconds. Find the temperature at $t = 480$ seconds using Euler's method. Assume a step size of $h = 240$ seconds.

Q2. Find an approximate value of

$$\int_5^8 6x^3 dx$$

using Euler's method of solving an ordinary differential equation. Use a step size of $h = 1.5$.

Q3. Repeat the problem 1 to find the temperature at $t = 480$ seconds using Runge-Kutta 2nd order method. Assume a step size of $h = 240$ seconds.

Q4. Repeat the problem 1 to find the temperature at $t = 480$ seconds using Runge-Kutta 4th order method. Assume a step size of $h = 240$ seconds.

Q5. Given $\frac{d^2y}{dt^2} + 2\frac{dy}{dt} + y = e^{-t}$, $y(0) = 1, \frac{dy}{dt}(0) = 2$, find by Euler's method

a) $y(0.75)$

b) the absolute relative true error for part(a), if $y(0.75)_{\text{exact}} = 1.668$

c) $\frac{dy}{dt}(0.75)$