

IIT ROPAR
SEMESTER I 2021-22
NUMERICAL SIMULATION LAB (CH230)
Assignment 2 Max Marks: 10

Note: Marks will be awarded for well written codes. Ensure that the files submitted are complete in all respects and only needed to be executed to get the required answers.

1. An enzyme behaves as a catalyst in a living cell. To represent enzyme-catalysed reactions, the Michaelis-Menten equation is widely used

$$r = \frac{a[S]}{b + [S]}$$

where

r is the reaction rate

$[S]$ denotes the concentration of the substrate S

a is the maximum initial reaction rate

b is a constant given by a combination of rate constants

The experimental data of reaction rates vs substrate concentrations is given below

$[S]$	1.2	1.6	3.2	4.3	5.8	7.6	8.8
r	0.06	0.12	0.24	0.27	0.33	0.34	0.34

Determine the parameters a and b in MATLAB using linear regression (by using a transformation to linearize this equation). What will be the reaction rate at $S = 2$ mg/L. Use an interpolation method to determine the reaction rate at $S = 2$ mg/L. Do you get the same value of r via the regression and interpolation methods?

On a single **well labelled** graph, indicate the experimental points (only the data points) and plot a smooth line plot of the equation obtained via linear regression and interpolation methods. **(6M)**

2. The absolute humidity (H) and dew point (DP) of air as a function of relative humidity is given below. Estimate H and DP when $RH = 58.4$ and T (dry bulb temperature) $= 46.8$ °C using cubic spline interpolation. **(4M)**

Relative Humidity (%RH)		10%	30%	50%	70%	90%
Dry bulb (°C)						
51	$H, \text{g/m}^3$	8.27	24.75	41.30	58.10	73.51
	$DP, ^\circ\text{C}$	10.10	26.89	37.01	43.21	47.80
44	$H, \text{g/m}^3$	6.52	19.58	32.70	45.75	58.78
	$DP, ^\circ\text{C}$	6.40	23.34	32.18	38.32	42.81