Name: ____________________________________

EXAM 2 - BIOE 391
Take Home – 2022

This portion of the exam is **open book/open notes**. Any other resources used must be acknowledged. Please **READ ALL INSTRUCTIONS**, manage your time effectively and answer the questions concisely but completely. Please upload a hard copy of the exam as a single PDF or Word file to Canvas. Handwritten formulas (equations) and diagrams are OK if the files are clearly scanned. Please make sure your file is clearly readable before uploading it. The recommended time investment in this take-home exam should be of no more than **5 hours**, although you are allowed to use more.

On my honor, I have neither given nor received any unauthorized aid on this exam.

Signature: _______________________

Read Carefully!

Please comment your code as much as possible. This will help us to grade and give YOU partial credit.

Problem 1 (30 pts). A Bioengineering team is studying chemical reactions describing the production, degradation, and interconversion of a cell-surface receptor that could exist in 4 states. Denoting the concentration of the receptor at each state (form) as $[X_i]$ (i=1,…,4), the following equations were formulated:

$$\begin{pmatrix} A(1-e^{-t}) \\ 0 \\ 0 \\ -1.9(1-e^{-2t}) \end{pmatrix} = \begin{pmatrix} -10 & 2 & k_1 & 1 \\ 8.99 & -7 & 2 & 1 \\ 1 & 5 & -3 & 0 \\ 0 & 0 & 0.5 & -2 \end{pmatrix} \begin{pmatrix} [X_1] \\ [X_2] \\ [X_3] \\ [X_4] \end{pmatrix} \qquad \text{(Equation 1)}$$

Here the vector on left-hand-side defines the time-dependent influx/efflux of the receptor forms; t is time in hours; k_1 is the rate constant.

a) Assuming A = 2 and $k_1 = 0.4$, write a MATLAB script, using the **Gauss-Seidel method**, to investigate how the receptor concentrations $[X_i]$ (i=1,..,4) at the four states depend on time t in the interval (0, 2.5) hours with the time step of 0.1 hours. Plot your solutions on the same graph. Assume tolerance $\epsilon_s = 1\%$.

b) Now, suppose the numerical solution differs from the measurements obtained, and the team attributed the discrepancy to the uncertainty in estimating k_1. Therefore, your next task is to investigate how the values of concentration for t=0.5 hours depend on k_1 (A is fixed at A=2). Develop a MATLAB function that takes k_1 as an input and returns a vector of four concentrations. Plot the solutions $[X_i]$ (i=1,..,4) vs k_1 for k_1 values between 0.3 and 0.5 (with 0.005 increment). Discuss your results in terms of the sensitivity of the solutions to changes in the rate constant k_1.

Problem 2 (20 pts). A bioengineering team designed a microfluidic chamber to test cell migration in the presence of a nutrient gradient. The diffusion reaction equation describing the concentration C(x) of the nutrient is:

$$C(x) = (x-1)^3 + 1 \qquad \text{(Equation 2)}$$

At one end of the tube (x = 0 mm) there is an absorbing reservoir that keeps the nutrient concentration at 0, where at the other end of the tube (x = 3.0 mm), there is a large source of nutrients that results in a fixed nutrient concentration of 9 mM.

a) Use an appropriate numerical method to compute the average concentration $\langle C \rangle$ of nutrient in the chamber, given by the following equation:

$$\langle C \rangle = \frac{1}{3.0}\int_0^{3.0} C(x)dx \qquad \text{(Equation 3)}$$

b) Justify your choice of integration method.

r	V(r)
0.2	0.4218
0.4	0.4747
0.6	0.5365
0.8	0.5714
1.0	0.5395
1.2	0.4219
1.4	0.2608
1.6	0.1175
1.8	0.0364
2.0	0.0073
2.2	0.0002

Table 1

Problem 3 (50 pts). As a part of bioengineering team working to develop artificial blood vessels to be implanted into patients, you are investigating radial velocity profile $V(r)$ of a viscoelastic liquid flowing through a tube of radius r. The measured $V(r)$ is given in **Table 1** (available on Canvas in excel format). Your goal is to determine the value r_0 for which $V(r_0) = 0.5$ using the following alternative approaches (plot your curve fitting results for each):

a) **Local cubic polynomial interpolation following by root finding:** Pick appropriate data points interpolate the data in the vicinity of the expected root with the cubic polynomial $p_3(r)$. Find the appropriate root of the equation $p_3(r) - 0.5=0$ using built-in MATLAB root-finding commands.

b) **Global cubic spline interpolation followed by root finding:** Using the whole data range in **Table 1**, use MATLAB built-in commands to define the spline interpolation function s(r) with <u>not-a-knot</u> end conditions. Find the appropriate root of the equation $s(r) – 0.5 = 0$ using built-in MATLAB root-finding commands.

c) **Generalized linear regression after logarithmic transformation:** Determine and apply an appropriate logarithmic transform to Equation 4. Use generalized linear regression to fit the log-transformed equation using the data given in **Table 1.** Convert the unknown coefficients back to Equation 4 after they are determined for the log-transformed equation. Use built-in MATLAB root-finding commands to the **largest positive root** of $V(r) = 0.5$. Plot your fitted curve with both a log and a linear y-axis for comparison with part (d).

$$V(r) = V_0 \exp\left(-\beta r^3 + \gamma r^2\right) \qquad \text{(Equation 4)}$$

d) **Non-linear regression following by root finding:** Based on the theoretical model you expect V(r) to be of the form of Equation 4. Use <u>non-linear least-square regression</u> to find the unknown coefficients V_0, β, and γ that minimizes the sum-of-squares error for the data given in Table 1. Use initial guesses based on your solution in (c). Once you have obtained the coefficients, use built-in MATLAB commands to find the **smallest positive root** of the equation $V(r) = 0.5$. Plot your fitted curve with both a log and linear y-axis for comparison with part (c).

e) Examine the fits produced by (c) and (d) and discuss which regression method is more appropriate, given the model and data.