

Assignment 4

Due date: **11:59 PM, November 15th, 2025**

Total: 20 Points

Instructions

- Make sure to submit fully executable Python scripts. You can submit a Jupyter Notebook (.ipynb) or a pure Python code (.py)
- Make an individual Jupyter Notebook or Python file for each question with the name question_<number>.ipynb/.py
- Zip all the relevant files and submit a single zipped folder with the name assign_3_<entry_number>.zip. This includes any modules that you wrote that the code imports.
- When you report the values of material properties either in text or on a plot, clearly mention the units.
- Spend time to make the plots look pretty by changing axis limits, labels and titles. The plots should be self-explanatory.
- Comment the code so I can follow your line of thought. This will help assign partial points in case you got the answer wrong.
- Few of the questions require you to comment on your findings. Use the markdown feature in Jupyter Notebook to write your comments. You can also use the multi-line comment feature in Python.
- In case of any anomalous or confusing statements in the assignments, use your best judgment and continue.
- These assignments are significant for mid-sem and final exams. Spend some time to understand and write the coding scripts.
- Submit the assignment on time. Late submissions will not be accepted.

Question-1: Modeling Hardness of Materials

Note: This is the same question as Q2 in Assignment 3. However, use ANN with hyperparameter tuning for both regression and classification here.

Modeling mechanical properties using machine learning is very extensive in material science. I have provided the "hardness_dataset.csv" which contains the experimental Hardness values (H_{exp}) for over 100 materials. Hardness as a material property is closely related to the modulus of the material. The dataset contains the bulk, shear, young modulus, and Poisson's Ratio. The hardness models should be trained on all four modulus features (including Poisson's Ratio). No feature selection is required. Answer the following questions, and make sure to read the full text of the question.

- (a) Perform Regression modeling using ANN to predict the material's experimental hardness values (H_{exp}). Perform hyperparameter tuning to find the model that gives the best metrics. Show results and clearly mention the best-trained model you have found and the metric used to make a determination.
- (b) Multiple constitutive relations are typically used to predict hardness from Modulus values. Some of them are as follows.

$$H1 = 0.1475 \times G \quad (1)$$

$$H2 = 0.0607 \times Y \quad (2)$$

$$H3 = 0.1769 \times G - 2.899 \quad (3)$$

$$H4 = 0.0635 \times Y \quad (4)$$

$$H5 = \frac{(1 - 2\nu)B}{6(1 + \nu)} \quad (5)$$

$$H6 = 2(k^2 G)^{0.585} - 3; k = G/B \quad (6)$$

For each data point, find the best equation that gives the closest hardness value to experiments (H_{exp}). Add that as the target column for the next question. You can use the absolute error between the H_{exp} and values predicted by the equation to determine the best relation for that data point. Also, mention each equation's average error of predictions and the best equation on average over the entire dataset. Note: All of these can be performed using pandas dataframes.

- (c) Next, perform classification modeling using ANNs to find the best model that predicts the best equation that should be used for a data point. As above, display the results from hyperparameter tuning and clearly indicate the best model and metric used for determination.

(10 points)

Question-2: Finite Difference Method

Suppose there was a block of Steel sandwiched between two blocks of Fe, as shown in the figure below. For simplicity, let's assume Carbon (C) is the only species diffusing in the system. The concentration at the beginning is 1 in the steel and 0 in the Fe. The boundary conditions on both ends of the system ($x = 0$ and 1) are Newmann BC's where the flux is zero.

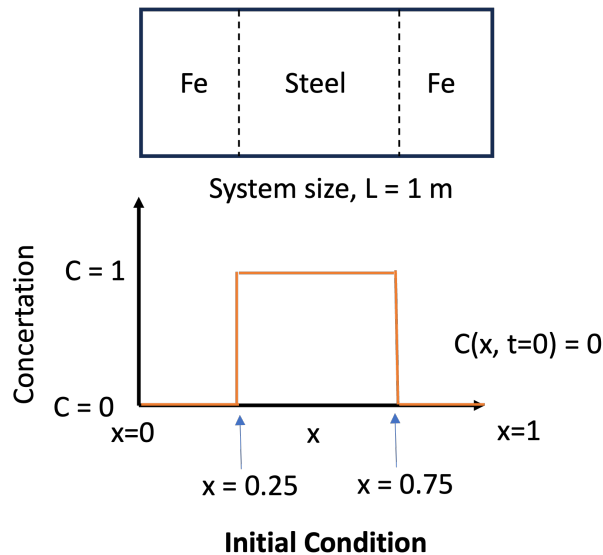


Figure 1: Initial conditions

Solve the concentration evolution in the following settings using the Finite Difference Method with the Implicit scheme. The total system size is $L = 1$ m.

- Consider the Diffusivity is constant $D = 1 \text{ m}^2/\text{s}$. Plot the evolution of the concentration until it reaches its final steady state.
- Now consider the Diffusivity is $D = 1.1 - x^2 \text{ m}^2/\text{s}$ where x is the distance from the origin. Plot the evolution of the concentration until it reaches its final steady state. Ensure that you use the Equation where diffusivity is not constant.
- Plot the concentration at the sandwich boundaries ($x = 0.25$ and 0.75) vs time until steady state. Each plot shows the concentration from the diffusivity cases in (a) and (b).
- Using the plots above, observe how diffusivity changes the concentration profile. What changed and what didn't?

(10 points)