Reading: Class notes: week 3.

Problems:

1. In Example 16 from the class note, we derived the least-squares solution for linear regression in the case of scalar real-valued inputs, $\{x^i: i=1,2,\ldots,N\}$, and outputs, $\{y^i: i=1,2,\ldots,N\}$, without a bias term. Now, we will extend this to include an additional bias weight, w_0 .

The linear regression model with a bias term is now given by:

$$y = wx + w_0$$

where w is the slope (weight) and w_0 is the bias.

1. Derive the updated least-squares cost function that includes the bias term w_0 . Show that the cost function to minimize is:

$$J(w, w_0) = \frac{1}{2N} \sum_{i=1}^{N} (y^i - (wx^i + w_0))^2$$

2. Compute the partial derivatives of $J(w, w_0)$ with respect to both w and w_0 . Verify that

$$\frac{\partial J}{\partial w} = -\frac{1}{N} \sum_{i=1}^{N} \left(y^i - (wx^i + w_0) \right) x^i$$

$$\frac{\partial J}{\partial w_0} = -\frac{1}{N} \sum_{i=1}^{N} \left(y^i - (wx^i + w_0) \right)$$

3. **Set the partial derivatives to zero** and obtain a system of simultaneous equations. Express the equations as

$$\begin{bmatrix} 1 & * \\ * & * \end{bmatrix} \begin{bmatrix} w_0 \\ w \end{bmatrix} = \begin{bmatrix} * \\ * \end{bmatrix}$$

4. Solve the system of equations to find the optimal values of w and w_0 . Show that the solution cana be expressed as follows:

$$w = \frac{\sum_{i=1}^{N} (x^i - \hat{x})(y^i - \hat{y})}{\sum_{i=1}^{N} (x^i - \hat{x})^2}, \quad w_0 = \hat{y} - w\hat{x}$$

where

$$\hat{x} = \frac{1}{N} \sum_{i=1}^{N} x^{i}, \qquad \hat{y} = \frac{1}{N} \sum_{i=1}^{N} y^{i}$$

[Hint: To solve the equations, it may be useful to first verify the following formula for inverse of a 2×2 matrix.

$$\begin{bmatrix} a & b \\ c & d \end{bmatrix}^{-1} = \frac{1}{ad - bc} \begin{bmatrix} d & -b \\ -c & a \end{bmatrix}, \quad (ad - bc) \neq 0$$

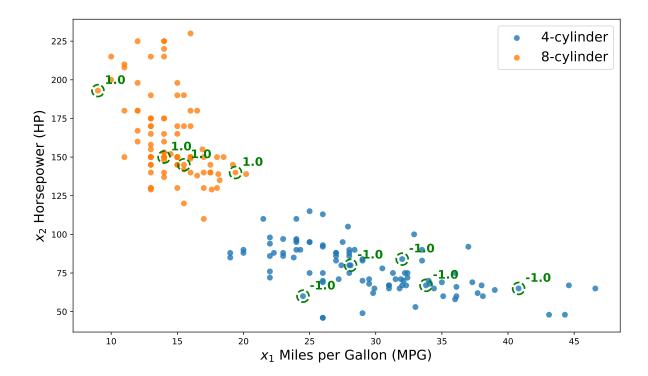


Figure 1: Scatter plot of the dataset. Each point represent a data sample with two features (x-axis and y-axis) and a category (color). The categories are represented by colors: blue (4-cylinder engines) and orange (8-cylinder engines).

The following questions are based on a dataset of vehicle characteristics that describes a relationship between miles per gallon (MPG), horsepower (HP), and the number of cylinders in the engine. The dataset and example Python scripts are provided, and can be accessed on GitHub.

- 2. Data Visualization and Interpretation: Examine the scatter plot (Figure 1) of the dataset:
 - 1. Describe the general features of data points. What might be the reason for such a distribution of data points? How many categories (labels) are there in the dataset? Is it possible to separate the categories?
 - 2. The green circles on data points indicate a few randomly selected samples. Run the Python code and read from terminal output to answer the following questions.
 - (a) What is the meaning of the green numbers for these highlighted data points? Note that these numbers are either 1 or -1?
 - (b) How many distinct samples N are there in the dataset?
 - 3. Create a mathematical model for this data-set as a single layer perceptron

$$y = \sigma(w^{\mathrm{T}}x)$$

- (a) What are the possible values of y? [Hint: These are related to the green numbers].
- (b) What is the form of x? [Hint: These are related to the two axes and a bias].
- (c) What is the choice of $\sigma(\cdot)$?

3. A binary classifier has been implemented using PyTorch to classify 4-cylinder and 8-cylinder engines. The decision boundary (separating the two categories) is given by

$$w^{\mathsf{T}}x = \begin{bmatrix} w_0 & w_1 & w_2 \end{bmatrix} \begin{bmatrix} 1 \\ x_1 \\ x_2 \end{bmatrix} = 0 \tag{1}$$

- 1. By inspection or trial and error, find one example of numerical values for w_0 , w_1 , w_2 that does not separate the dataset.
- 2. By inspection or trial and error, find one example of numerical values for w_0 , w_1 , w_2 that does separate the dataset.
- 3. Turn in a plot showing the two decision boundaries with the incorrect and the correct choice.
- 4. For each choice, compute and report the resulted value of the loss function

$$J(w_0, w_1, w_2) = \frac{1}{2N} \sum_{i=1}^{N} (y^i - (w_1 x_1^i + w_2 x_2^i + w_0))^2$$

- 4. Least square algorithm: A code has been provided to implement the least squares algorithm
 - 1. Run the code to obtain the optimal decision boundary.
 - 2. Does the optimal weight vector obtained by the least squares algorithm separate the two groups (4-cylinder and 8-cylinder engines)?
 - 3. Turn in a plot showing the optimal decision boundary. Report the numerical value of the optimal weights.
 - 4. Report the numerical value of the loss. Compare with the numerical value of the loss for your two choices in Problem 3.