CS5785 Homework 1

The homework is generally split into programming exercises and written exercises.

This homework is due on **September 16, 2021 at 11:59 PM EST**. Upload your homework to **Gradescope**. There are two assignments for this homework in Gradescope. Please note a complete submission should include:

- 1. A write-up as a single .pdf file, which should be submitted to "Homework 1 (write-up)" This file should contain your answers to the written questions **and** exported pdf file / structured write-up of your answers to the coding questions (which should include core codes, plots, outputs, and any comments / explanations).
- 2. Source code for all of your experiments (AND figures) zipped into a single .zip file, in .py files if you use Python or .ipynb files if you use the IPython Notebook. If you use some other language, include all build scripts necessary to build and run your project along with instructions on how to compile and run your code. If you use the IPython Notebook to create any graphs, please make sure you also include them in your write-up. This should be submitted to "Homework 1 (code)".

The write-up should contain a general summary of what you did, how well your solution works, any insights you found, etc. On the cover page, include the class name, homework number, and team member names. You are responsible for submitting clear, organized answers to the questions. You could use online Later templates from Overleaf, under "Homework Assignment" and and "Project / Lab Report".

Please include all relevant information for a question, including text response, equations, figures, graphs, output, etc. If you include graphs, be sure to include the source code that generated them. Please pay attention to Slack for relevant information regarding updates, tips, and policy changes. You are encouraged (but not required) to work in groups of 2.

IF YOU NEED HELP

There are several strategies available to you.

- If you get stuck, we encourage you to post a question on the Discussions section of Canvas. That way, your questions/solutions will be available to other students in the class.
- Your instructor and TAs will offer office hours, which are a great way to get some one-on-one help.
- You are allowed to use well known libraries such as scikit-learn, scikit-image, numpy, scipy, etc. in this assignment. Any reference or copy of public code repositories should be properly cited in your submission (examples include Github, Wikipedia, Blogs).

PROGRAMMING EXERCISES

Please use different .py or .ipynb files for different parts

Part I. The Housing Prices

- 1. Join the House Prices Advanced Regression Techniques competition on Kaggle. Download the training and test data.
- 2. Give 3 examples of continuous and categorical features in the dataset; choose one feature of each type and plot the histogram to illustrate the distribution.
- 3. Pre-process your data, explain your pre-processing steps, and the reasons why you need them. (Hint: data pre-processing steps can include but are not restricted to: dealing with missing values, normalizing numerical values, dealing with categorical values etc.)
- 4. One common method of pre-processing categorical features is to use a one-hot encoding (OHE).

Suppose that we start with a categorical feature x_j , taking three possible values: $x_j \in \{R, G, B\}$. A one-hot encoding of this feature replaces x_j with three new features: x_{jR}, x_{jG}, x_{jB} . Each feature contains a binary value of 0 or 1, depending on the value taken by x_j . For example, if $x_j = G$, then $x_{jG} = 1$ and $x_{jR} = x_{jB} = 0$.

Give some examples of features that you think should use a one-hot encoding and explain why. Convert at least one feature to a one-hot encoding (you can use your own implementation, or that in pandas or scikit-learn) and visualize the results by plotting feature histograms of the original feature and its new one-hot encoding.

- 5. Using ordinary least squares (OLS), try to predict house prices on this dataset. Choose the features (or combinations of features) you would like to use or ignore, provided you justify your choice. Evaluate your predictions on the training set using the MSE and the R^2 score. For this question, you need to implement OLS from scratch without using any external libraries or packages.
- 6. Train your classifier using all of the training data, and test it using the testing data. Submit your results to Kaggle.

Part II. The Titanic Disaster

- 1. Join the Titanic: Machine Learning From Disaster competition on Kaggle. Download and preprocess the data.
- 2. Using logistic regression, try to predict whether a passenger survived the disaster. Choose the features (or combinations of features) you would like to use or ignore, provided you justify your choice.
- 3. Train your classifier using all of the training data, and test it using the testing data. Submit your results to Kaggle.

WRITTEN EXERCISES

1. Maximum Likelihood and KL Divergence. In machine learning, we often need to assess the similarity between pairs of distributions. This is often done using the Kullback-Leibler (KL) divergence:

$$KL(p(x)||q(x)) = \mathbb{E}_{p(x)} \left[\log p(x) - \log q(x) \right]$$

The KL divergence is always non-negative, and equals zero when p and q are identical. This makes it a natural tool for comparing distributions.

This question explores connections between the KL divergence and maximum likelihood learning. Suppose we want to learn a supervised probabilistic model $p_{\theta}(y|x)$ (e.g., logistic regression) with parameters θ over a dataset $\mathcal{D} = \{(x^{(i)}, y^{(i)}) \mid i = 1, 2, ..., n\}$. Let $\hat{p}(x, y)$ denote the *empirical* distribution of the data, which is the distribution that assigns a probability of 1/n to each of the data points in \mathcal{D} (and zero to all the other possible (x, y)):

$$\hat{p}(x, y) = \begin{cases} \frac{1}{n} & \text{if } (x, y) \in \mathcal{D} \\ 0 & \text{otherwise.} \end{cases}$$

The empirical distribution can be seen as a guess of the true data distribution from which the dataset \mathcal{D} was sampled i.i.d.: it assigns a uniform probability to every possible training instance seen so far, and does not assign any probability to unseen training instances.

Prove that selecting parameters θ by maximizing the likelihood is equivalent to selecting θ that minimize the average KL divergence between the data distribution and the model distribution:

$$\arg\max_{\theta} \mathbb{E}_{\hat{p}(x,y)} \left[\log p_{\theta}(y|x) \right] = \arg\min_{\theta} \mathbb{E}_{\hat{p}(x)} \left[KL(\hat{p}(y|x)||p_{\theta}(y|x)) \right].$$

Here, $\mathbb{E}_{p(x)}f(x)$ denotes $\sum_{x \in \mathcal{X}} f(x)p(x)$ if x is discrete and $\int_{x \in \mathcal{X}} f(x)p(x)dx$ if x is continuous.

- 2. Gradient and log-likelihood for logistic regression.
 - (a) Let $\sigma(a) = \frac{1}{1 + e^{-a}}$ be the sigmoid function. Show that $\frac{d\sigma(a)}{da} = \sigma(a) (1 \sigma(a))$.
 - (b) Using the previous result and the chain rule of calculus, derive the expression for the gradient of the log likelihood:

$$\nabla L(\theta) = [\sigma(\theta^T \mathbf{x}) - y]\mathbf{x}$$

where

$$L(\theta) = -\left[y\log\sigma(\theta^T\mathbf{x}) + (1-y)\log(1-\sigma(\theta^T\mathbf{x}))\right]$$

3. Linear regression and OLS. Consider the following two-dimensional dataset consisting of seven data points:

$$(-1,-1), (-1,0), (0,-1), (0,0), (0,1), (1,0), (1,1)$$

(a) Plot the seven data points. Without performing any calculations, what do you think is the result of fitting a linear model to this dataset using the MSE (i.e., what is the slope and intercept of the best fit line)?

- (b) Calculate the slope and the intercept of a linear model fit to this dataset using the MSE. Explain your answer via a mathematical argument or via code that computes the model parameters. If the answer is different from what you wrote in (a), comment on why that's the case.
- (c) Calculate the slope and the intercept of a linear model fit to this dataset using the *mean absolute error* (i.e., the L1 loss). Briefly explain how you obtained your answer and comment on the result.