Homework 2

Instructions on homework submission. Please upload your solutions to Gradescope. You need to use this template for your written submission. You may use LaTeX or print the template and hand-write your answers then scan it in. Failure to use the template may result in a penalty. Handwritten submissions should be clearly legible. If your writing is not legible, you will not be awarded marks. Please make sure your answers are fully included in the given space for each question.

Instructions on programming assignments. You need to submit your code for Question 2 and for Question 4 in the Homework 2 (programming) section on gradescope.

For Question 2, your submission will be graded by Autograder. Follow the detailed instruction in Question 2.

For Question 4, the plots generated by your code needs to be in the pdf file (written submission). However, **your answers for Question 4 in the written submission will not be graded if you do not submit the codes in the programming part.** You are required to use Python as the programming language. Please submit your .py file or .ipynb file as submission with instructions on how to execute your code.

For the integrity and conciseness of grading, please ask questions to:

Young Je: Problem 1, Problem 2, Problem 3

Parker: Problem 4

1. [Logistic Regression, Theory 20 pts] Consider the following logistic regression model for two-class classification

$$P(Y=1|X) = \frac{1}{1+\exp(w_0 + w_1 X_1 + w_2 X_2)}$$

for classifying the data in Figure 1.

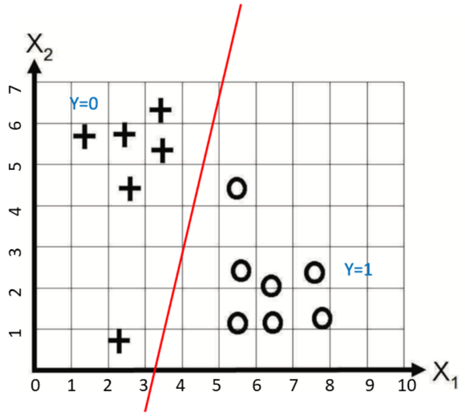
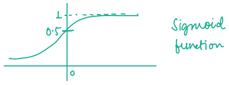


Figure 1: Training data

(a) [2 pts] Find the training sample with the highest probability of class 1. Find the training sample with the highest probability of class 0. You may specify the sample using coordinates or the value range of X_1 and X_2. Provide brief justification of your answer.

Training Sample with the highest probability of class 1 is (7.9, 1.2)
Training Sample with the highest probability of class 0 is (1.2, 5.8)
On the sigmoid function, point (7.9, 1.2) will be found near 1 on the y-axis and point (1.2, 5.8) will be found near 0 on the y-axis.



(b) [5 pts] Use a linear equation to describe the decision boundary (red line) in Figure 1.

$w_1 x_1 + w_2 x_2 + w_0 = 0$

(c) [3 pts] Consider modifying this classifier so that it uses only feature X_1. Provide the equation for this decision boundary. Consider modifying this classifier so that it uses only feature X_2. Provide the equation for this decision boundary. Which of the two classifiers will perform better on the training data? Provide justification.

only using feature X_1: $w_0 + w_1 x_1 = 0$; only using feature X_2: $w_0 + w_2 x_2 = 0$
The classifier using only feature X_1 will perform better on the training data because the decision boundary along the X_1 axis better separates the data into two classes ($Y=1, Y=0$) whereas the decision boundary along the X_2 axis does not completely distinguish the data points into two classes ($Y=0, Y=1$) as there remains one or two data points in the wrong class when a decision boundary is drawn along the X_2 axis.

(d) [5 pts] Consider using decision tree on the data in Figure 1, instead of logistic regression. What is the advantage and disadvantage of decision tree over logistic regression?

Advantage: Decision trees are non linear classifiers and therefore don't need data to be separated linearly. Also accounts for interactions between different Variables / features.

Disadvantage: Decision trees require higher time to train the model. Additionally, a minute change in the data can lead to a large change in the tree structure. It is also relatively expensive.

(e) [5 pts] Consider using Naive Bayes classifier and decision tree on the data in Figure 1. What is the advantage and disadvantage of Naive Bayes over logistic regression?

Advantage: Naive Bayes classifier has a higher bias and low variance which makes it easier to make predictions with less Variables / features and less data

Disadvantage: Naive Bayes classifier expects the features to be independent which is not always true.

2. [Logistic Regression, Implementation 10 pts] This problem is graded with Autograder. Follow the below instruction, and implement in **reg.py**.
Do not rename this files, and do not change anything other than the functions you are asked to implement. Otherwise, Autograder might unable to grade your work properly. You are only allowed to use Numpy in this problem.

In this part, you need to train a linear binary classification model $F(x) = \langle w, x \rangle$ with logistic regression (for simplicity, the bias term b is omitted here). For training samples $\{(x_i, y_i)\}_{i=1}^n$ where $x_i \in \mathbb{R}^d$ and $y_i \in \{0, 1\}$, you need to find a vector $w \in \mathbb{R}^d$ that minimizes the following loss function:

$$\ell(w) = \frac{1}{n} \sum_{i=1}^{n} \left[\log(1 + e^{\langle w, x_i \rangle}) - y_i \cdot \langle w, x_i \rangle \right]$$

which is the negative log likelihood. Minimizing this loss function is a convex optimization problem, which means that in most cases, there exists a unique minimizer. Here, you need to find this minimizer with gradient descent, which runs as follows:

```
**Algorithm 1** Gradient Descent
**Require:** Learning rate $\eta > 0$, stopping criterion $\rho > 0$
  Initialize $w$
  **while** True **do**
      Compute gradient $\nabla_w \ell(w)$
      If $\|\nabla_w \ell(w)\| < \rho$ then break
      $w \leftarrow w - \eta \cdot \nabla_w \ell(w)$
  **end while**
```

Task: In `reg.py`, implement three functions: `compute_loss` for computing $\ell(w)$, `compute_grad` for computing $\nabla_w \ell(w)$, and `train` for training the model with gradient descent.

3. [Decision Tree, 20 pts] A group of students ran several experiments to design a system to determine the effectiveness of initial drug screening campaign. Your friend took notes on the 8 experiments he has ran, and he wants to construct a decision tree that would predict whether or not drug has effect based on 3 binary features:

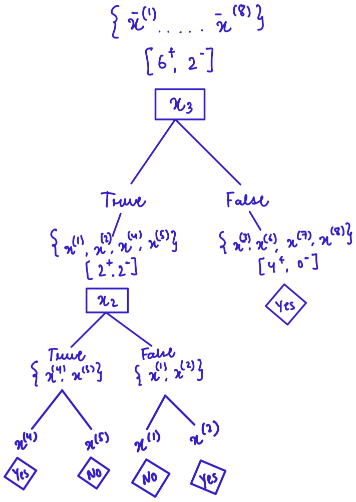
   - x_1 = The drug molecule has benzene ring
   - x_2 = The drug molecule has more than 2 negative ions
   - x_3 = The drug molecule showed less than 2 angstrom distance from pocket

Movie	x_1	x_2	x_3	Like
$\bar{x}^{(1)}$	False	False	True	No
$\bar{x}^{(2)}$	True	False	True	Yes
$\bar{x}^{(3)}$	False	False	False	Yes
$\bar{x}^{(4)}$	False	True	True	Yes
$\bar{x}^{(5)}$	True	True	True	No
$\bar{x}^{(6)}$	True	False	False	Yes
$\bar{x}^{(7)}$	True	True	False	Yes
$\bar{x}^{(8)}$	False	True	False	Yes

   (a) [5 pts] Use the above dataset to construct a decision tree, where each split is performed on the feature with the highest information gain. Use the following stopping conditions in the decision tree algorithm:

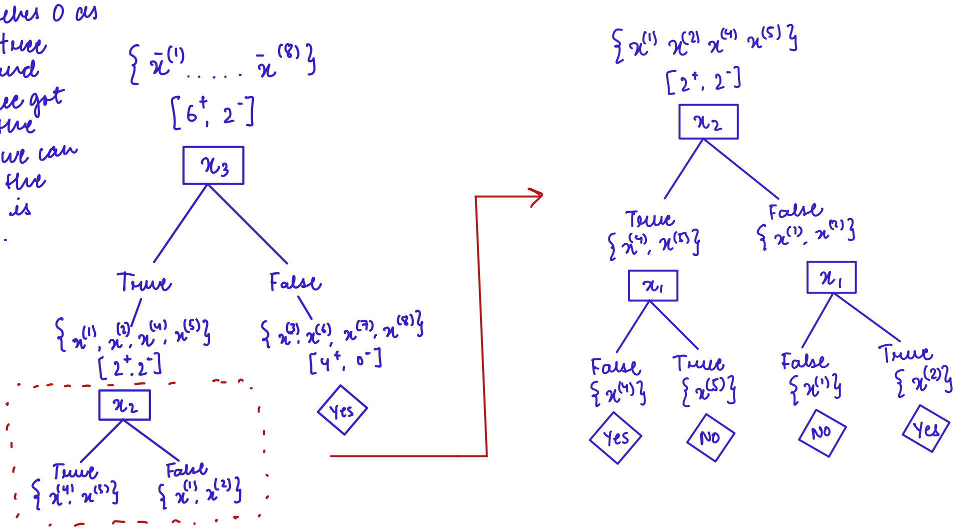
   - Tree depth is 3
   - Information gain is 0

Output majority label if any of the stopping criteria are met, or a positive label if both classes are equally represented. **NOTE**: To help you out, the TAs have decided to tell you that the split at the root made by this algorithm will be on the feature x_3.



(b) [5 pts] Does your decision tree from previous part minimize the training error? If not, report the smallest training error that a decision tree can achieve on this dataset and draw the decision tree.

No, the decision tree from previous part does not minimize the training error. The training error approaches 0 as the decision tree gets bigger and since the tree got bigger from the previous part, we can assume that the training error is approaching 0.



(c) [10 pts] During recitation, we introduced KL-Divergence to provide another view of information gain. Here we have formal definition of KL-Divergence:

Let p and q be two discrete probability distributions defined over the same event space. Formally, for $i \in \{1, ..., n\}$, let $p(i)$ be the probability of event i occurring under distribution p and $q(i)$ be the corresponding probability under distribution q. The **Kullback-**

Leibler (KL) divergence between p and q is defined as

$$D(p\|q) = \sum_{i=1}^{n} p(i) \log \frac{p(i)}{q(i)}$$

KL-Divergence is proven to have non-negative: $D(p\|q) \geq 0$. Using this, we want to show that information gain is always non-negative. In detail,

In a sample S, the information gain of a variable Y with respect to a target variable X is the expected reduction in entropy of a target variable X after gaining insight into Y:

$$Gain(S, Y) = H_S(X) - H_S(X \mid Y)$$

Show that information gain is always non-negative. Show all steps of your work.

$H_S(X|Y) = \sum_{v} P(Y=v) H(X|Y=v) = \sum_{v} P(Y=v)\left(-\sum_{i=1}^{n} P(X=i|Y=v) \log_2 P(X=i|Y=v)\right) = -\sum_{v}\sum_{i=1}^{n} P(X=i, Y=v) \log_2 P(X=i|Y=v)$

$H(X) = -\sum_{i=1}^{n} P(X=i) \log_2 P(X=i)$; So, $H_S(X) - H_S(X|Y) = \sum_{v}\sum_{i=1}^{n} P(X=i, Y=v) \log_2 P(X=i|Y=v) - \sum_{i=1}^{n} P(X=i) \log_2 P(X=i)$

Now, $\sum_{i=1}^{n} P(X=i) \log_2 P(X=i) = \sum_{v}\sum_{i=1}^{n} P(X=i, Y=v) \log_2 P(X=i|Y=v)$

$\Rightarrow H_S(X) - H_S(X|Y) = \sum_{i=1}^{n}\sum_{v} P(X=i, Y=v)\left(\log_2 P(X=i|Y=v) - \log_2 P(X=i)\right) \log_2 P(X=i|Y=v) - \log_2 P(X=i)$

$= \log_2 \frac{P(X=i, Y=v)}{P(Y=v)} - \log_2 P(X=i) = \log_2 \frac{P(X=i, Y=v)}{P(Y=v, X=i)}$

Thus, $H_S(X) - H_S(X|Y) = \sum_{v}\sum_{i=1}^{n} P(X=i, Y=v) \log_2 \frac{P(X=i, Y=v)}{P(Y=v, X=i)}$;

Now, $\sum_{v}\sum_{i=1}^{n} P(X=i, Y=v) = 1$

$\Rightarrow \sum_{v}\sum_{i=1}^{n} P(X=i) P(Y=v) = \sum_{v} P(Y=v) = 1$

So, we can see $\{P(X=i, Y=v)\}_{1 \leq i \leq v}$ & $\{P(X=i) P(Y=v)\}_{1 \leq i \leq v}$ as different probability distributions on same event space which is (event space of X × event space of Y).

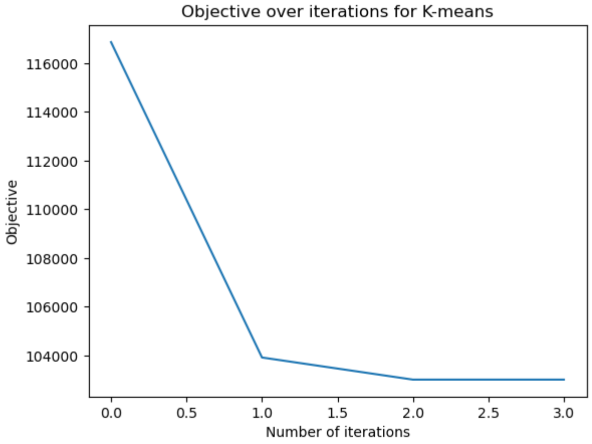
By KL divergence, we have

$\sum_{v}\sum_{i=1}^{n} P(X=i, Y=v) \log_2 \frac{P(X=i, Y=v)}{P(X=i) P(Y=v)} \geq 0 \Rightarrow$ So, $H_S(X) - H_S(X|Y) \geq 0$

4. [K-Means Clustering, 50 pts] In this homework problem, you will implement K-means algorithm and apply it to cluster genes using the mouse gene expression data from three brain tissue types, HIP, PFC, and STR. For each tissue type, data are provided in two files, one for expression data, where the rows are for mice/samples and the columns are for genes, and the other file for gene names. Answer the following questions on the tissue type HIP. Exlore PFC and STR in the bonus problem.

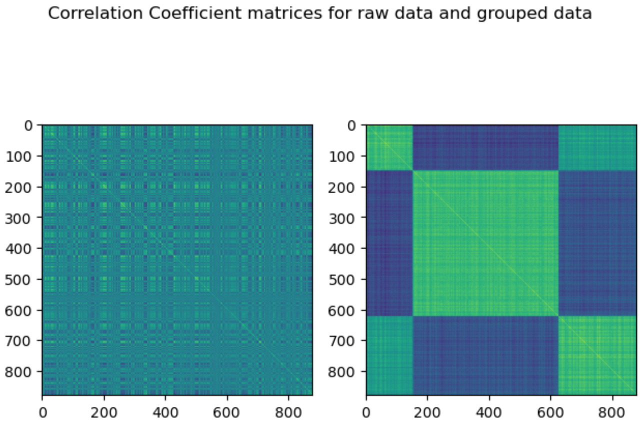
   Note: For ploting the correlation coefficient matrix you can use the pyplot function imshow(). For parts (c) and (d) you should show all the correlation coefficient matrices in one plot. You can achieve this with the pyplot.subplots() function. Each subplot should be titled with the objective function value (parts (c) and d) and the K value (part (d) only).

   (a) [15 pts] Run K-means algorithm with $K = 3$ with the initialization of K means given in 'test_mean.txt'. Plot the objective (y-axis) over iterations (x-axis). What is the objective value at convergence? (Make sure you use the given initialization. The initialization is given for the grading purpose.)



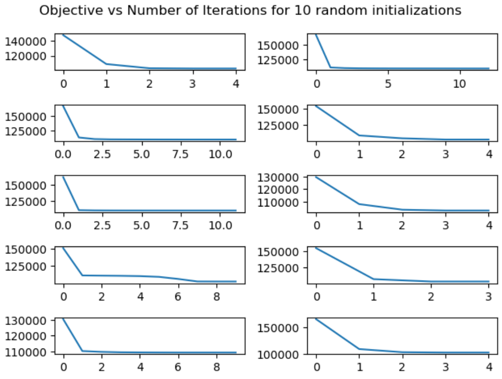
The objective value at convergence is 103010.60.

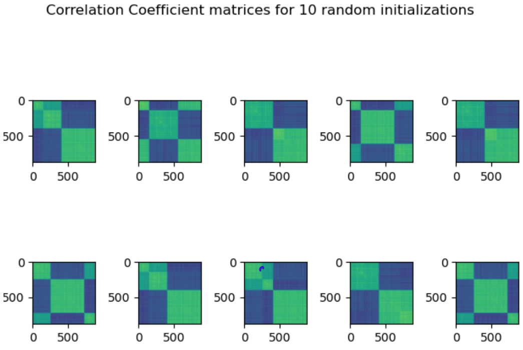
(b) [10 pts] Run K-means algorithm with $K = 3$ with your own random initialization. Plot the correlation coefficient matrix of a) the raw data and b) the data after you group the columns of the expression matrix according to the clusters found by K-means. Plot these as an image of $N \times N$ correlation matrix for N genes.



(c) [10 pts] With $K = 3$, try 10 random initializations. Show the correlation coefficient matrix as above and the corresponding objective at convergence for each initialization. Which of the 10 results would you choose for follow-up analysis?

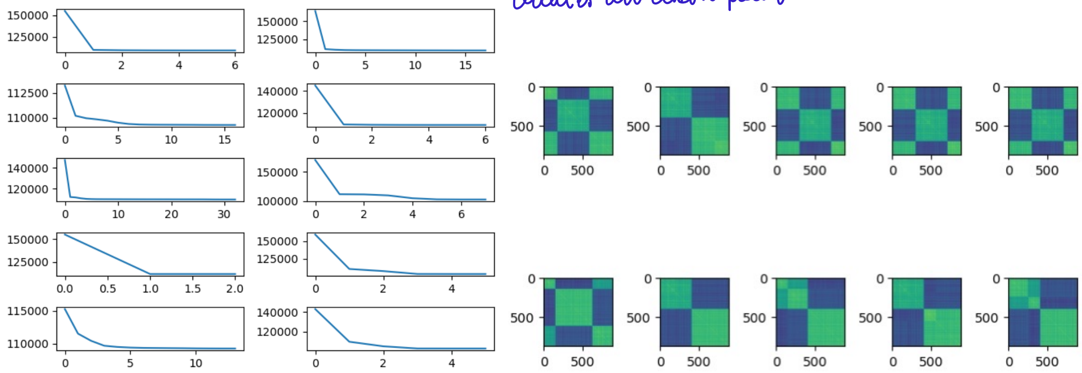
Out of the 10 results, I would choose the one with the lowest objective value for follow up analysis which is 103010.60.





(d) [15 pts] Run K-means algorithm for $K = 3, \ldots, 12$, with 10 random initializations for each K. Show the correlation coefficient matrix and objectives at convergence for different K, with your best choice of the 10 runs for each K. What do you think is the best K? Why?

The best choice of K is one with the sharpest drop to reach convergence in the plot of objective function because that's the one where distortion declines the most and creates an elbow point.



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