18-661: Introduction to ML for Engineers

Final Review

Spring 2025

ECE – Carnegie Mellon University

Logistic Regression

Question: Training a logistic regression model for binary classification is equivalent to training a two-layer neural network with one linear layer and one softmax layer.

- ○ True
- ○ False

Logistic Regression

True. Logistic regression models the probability of a data point belonging to each class as the sigmoid function of a linear combination of the input features, which is exactly what a linear layer plus softmax layer does for binary classification.

Decision Trees

Question: In decision tree algorithms, including attributes that have no direct effect on the target variable can be beneficial for the robustness of the learned model because they add complexity that can capture unforeseen patterns.

- ○ True
- ○ False

Decision Trees

False. Including attributes that do not affect the target variable tends to add unnecessary complexity to the model, which can lead to over-fitting by capturing noise rather than meaningful patterns. The robustness of a decision tree model is improved by including relevant attributes that contribute to information gain, not by the indiscriminate addition of complexity.

Clustering

Question: The K-means clustering algorithm is guaranteed to converge if it does not encounter any ties in the distance of a point from the cluster centers.

- ○ True
- ○ False

Clustering

True.

Distributed Learning

Question: Consider using synchronous distributed SGD (stochastic gradient descent) to train a linear regression model, where the data is shuffled and uniformly distributed across m workers. The expected error (i.e., ℓ_2 loss) after t iterations of synchronous distributed SGD with m workers and a batch size of b per worker is equivalent to the expected error of single-worker mini-batch SGD with a batch size of mb after t iterations.

- ○ True
- ○ False

True. In both scenarios, we are effectively performing gradient descent on *mb* data points chosen uniformly at random from the entire training dataset.

Bandits

Question: A Markov Decision Process (MDP) becomes equivalent to the multi-armed bandit formulation when we set the discount factor to $\gamma = 0$, there is a single state without any state transitions, and the reward function is only action dependent (i.e. the reward is given by $r(a)$ where a represents the action).

- ◦ True
- ◦ False

Bandits

True.

KNN

Question: You are building a k-nearest neighbors model to predict students' final grades based on their study hours, attendance rate, midterm grades, and assignment grades. From earlier knowledge, you know that assignment grades are the most important indicator. After training your model with a certain dataset, you realize that it performs well on the training set but poorly on the test set. Which of the following steps is most likely to improve the generalization performance of your k-nearest neighbors model?

- ○ Increase the value of k.
- ○ Decrease the value of k.
- ○ Remove the assignment grades feature.
- ○ Replace the Euclidean distance (L2-norm) with the Manhattan distance (L1-norm).

KNN

A. Increasing k will decrease the variance, helping to prevent overfitting to the training dataset.

Bias-Variance Tradeoff

Question: Suppose you train a neural network on a training dataset $\mathcal{D}_T$, using a validation dataset $\mathcal{D}_V$ to determine the optimal value of the model hyperparameters. However, you observe that while the trained neural network has low training error, it has high testing error on the test dataset. Which of the following mistakes in your training procedure might explain these results?

- ◦ You accidentally omitted half of the training data.
- ◦ You accidentally used the same training and validation datasets (i.e., $\mathcal{D}_V$ was mistakenly set to be the same as $\mathcal{D}_T$).
- ◦ You used a neural network with too many layers.
- ◦ All of the above.

Bias-Variance Tradeoff

D. Omitting half of the training data makes the model more likely to overfit to the training dataset. Using the training data as validation also makes the model prone to overfitting. Using a neural network that is too deep can also lead to overfitting.

Clustering

Question: You want to perform K-means clustering on a dataset of N social network users to identify groups of similar users. You are not sure what is the right value of K, so you decide to plot the final value of the cost function J when using K clusters versus K for all K in the range 1 to N. Recall that

$$J = \sum_{n=1}^{N} \sum_{k=1}^{K} r_{nk} \|\boldsymbol{x}_n - \boldsymbol{\mu}_k\|^2.$$

where $\boldsymbol{x}_n$ is the feature vector of the n-th sample, $\boldsymbol{\mu}_k$ is the k-th cluster mean and r_{nk} is 1 if sample n is assigned to cluster k and 0 otherwise.

Which of the following statements is TRUE?

- ○ J decreases or stays the same as K increases. The optimal K is the smallest possible value.
- ○ J first decreases and then increases with K. The optimal K is the one that minimizes J.
- ○ J first increases and then decreases with K. The optimal K is the one that maximizes J.
- ○ None of the above.

Clustering

D. J decreases or stays the same as K increases, but the best K is at the 'elbow' of the function.

Distributed Learning

Question: Consider a distributed SGD implementation with m workers with a mini-batch size b per worker. Suppose that each worker takes exponential time rate μ (and mean $1/\mu$) to finish its mini-batch gradient computation, and that these times are independent across workers and mini-batches. What are the expected times taken by synchronous and asynchronous SGD to finish processing N mini-batches of data?
[Hint:] The expected minimum and maximum of n independent exponential random variables with rate μ are $\frac{1}{n\mu}$ and $\frac{\log n}{\mu}$ respectively.

- Sync SGD $= \frac{N \log m}{\mu}$, Async SGD $= \frac{N}{m\mu}$
- Sync SGD $= \frac{N\mu}{\log m}$, Async SGD $= \frac{Nm}{\mu}$
- Sync SGD $= \frac{N \log m}{\mu}$, Async SGD $= \frac{Nm}{\mu}$
- Sync SGD $= \frac{Nm \log m}{\mu}$, Async SGD $= \frac{N}{m\mu}$

A. The time taken to complete one iteration of synchronous SGD in which we process m mini-batches is $\log m/\mu$, and thus the time to process N mini-batches is $N \log m/\mu$. The time taken to complete one iteration of asynchronous SGD in which we process 1 mini-batch is $1/m\mu$, and thus the time to process N mini-batches is $N/m\mu$.

Nearest Neighbors

Question: Consider a dataset containing the following three 2-dimensional points along with their corresponding labels (y-values) as shown below.

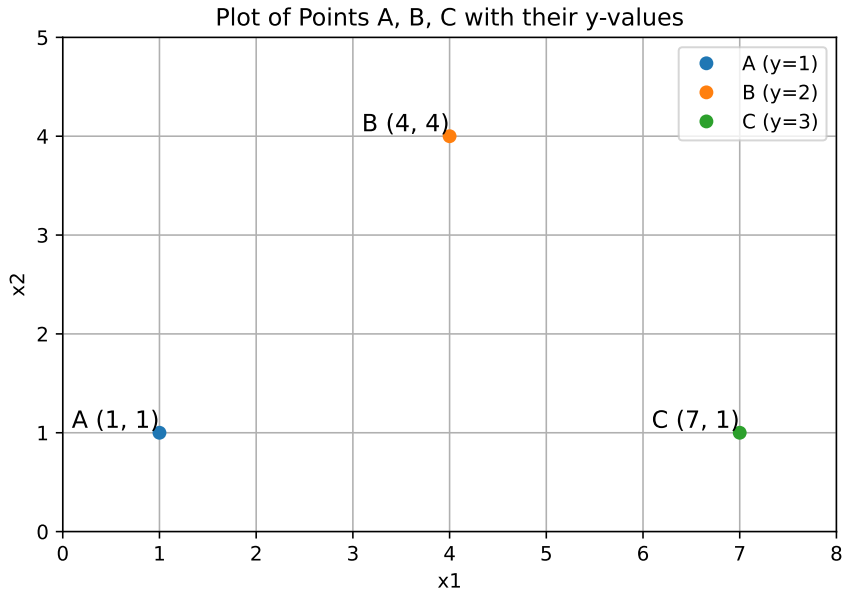


Figure 1: Dataset for Problem 17.

Point A: $(x_1 = 1, x_2 = 1)$, $y = 1$
Point B: $(x_1 = 4, x_2 = 4)$, $y = 2$
Point C: $(x_1 = 7, x_2 = 1)$, $y = 3$

Nearest Neighbors

Suppose that you perform k-Nearest Neighbors regression for predicting the y-value, $\hat{y}$, with $k = 1$ and with the Euclidean distance (i.e., ℓ_2 distance) metric. For any new point (x_1, x_2) we want to find the decision regions for all possible $\hat{y}$ in terms of x_1 and x_2.

Draw the decision boundaries on the figure.

Specify the decision region in which we predict label $\hat{y} = 1$ for a point (x_1, x_2).

Specify the decision region in which we predict label $\hat{y} = 2$ for a point (x_1, x_2).

Specify the decision region in which we predict label $\hat{y} = 3$ for a point (x_1, x_2).

Nearest Neighbors

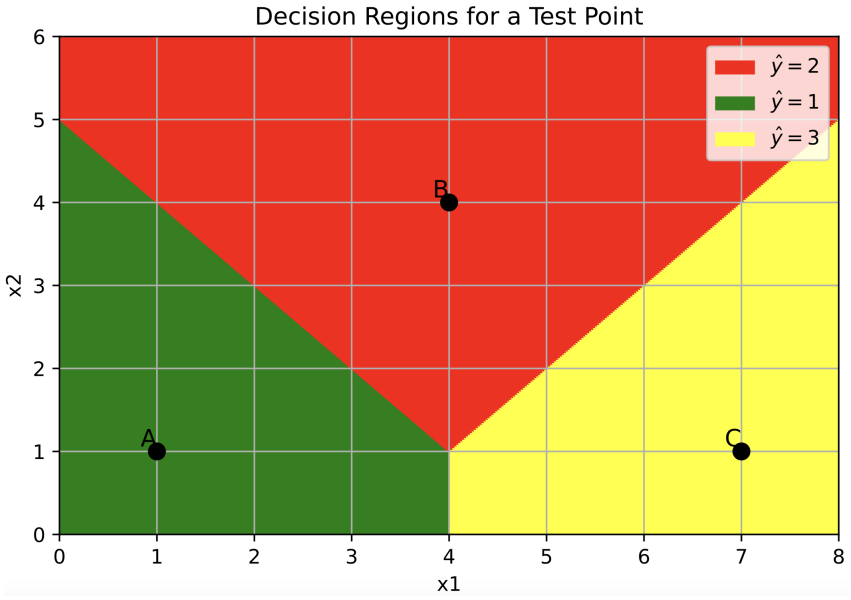


Figure 2: Problem 5 Solution Figure

Then, we can have the following decision rules

- $\hat{y} = 2$ if $\{x_1 + x_2 > 5$ and $x_1 - x_2 < 3\}$ by using (2.) and (3.)
- $\hat{y} = 1$ if $\{x_1 < 4$ and $x_1 + x_2 \leq 5\}$ by using (1.) and (2.)
- $\hat{y} = 3$ if $\{x_1 \geq 4$ and $x_1 - x_2 \geq 3\}$ by using (2.) and (3.)

PCA

Question: Suppose you are given a dataset $\mathcal{D}$ of N data points, where N is an even number and $\mathcal{D} = \left\{ (-1)^j \left\lceil \frac{j}{2} \right\rceil \begin{bmatrix} 1 \\ -1 \\ 0 \end{bmatrix}, j = 1, 2, \ldots, N \right\}$.

Each data point therefore has three input features.

Note that the notation $\lceil \alpha \rceil$ refers to the smallest integer greater than or equal to α. For example, $\lceil \frac{1}{2} \rceil = 1$.

PCA

Question: Let $N = 2$, so that $\mathcal{D} = \left\{ \begin{bmatrix} 1 \\ -1 \\ 0 \end{bmatrix}, \begin{bmatrix} -1 \\ 1 \\ 0 \end{bmatrix} \right\}$. Suppose you run PCA (principal component analysis) to find the top principal component on this dataset. What principal component do you find?

PCA

The top principal component is $\frac{\sqrt{2}}{2}\begin{bmatrix}1\\-1\\0\end{bmatrix}$. One can see this directly from the dataset, as this principal component leads to zero reconstruction loss. Alternatively, one can see that all variance in this dataset occurs along this vector, which therefore should be the principal component.

Mathematically, our data is zero-centered, so the covariance matrix $X^TX = \begin{bmatrix}2 & -2 & 0\\-2 & 2 & 0\\0 & 0 & 0\end{bmatrix}$; it is easy to see that the only nonzero eigenvalue of this matrix is 2, with associated eigenvector $\begin{bmatrix}1\\-1\\0\end{bmatrix}$.

PCA

Question: Now suppose that $N = 4$, and that you again run PCA to find the top principal component on $\mathcal{D}$. What principal component do you find? Is it the same as the one you found in part (a) for $N = 2$? Briefly explain your answer.

We obtain the same answer as in part (a). All variation in our dataset still occurs along the same vector $\begin{bmatrix} 1 \\ -1 \\ 0 \end{bmatrix}$, as each vector is a multiple of this vector, and therefore the same reasoning as in part (a) holds.

PCA

Question: You are now asked to find the top *two* principal components for the dataset in part (b). Will this lead to a decrease in the average reconstruction error over the data points in $\mathcal{D}$, compared to the reconstruction error with the single principal component you found in part (b)? Briefly explain your answer.

Recall that the *reconstruction error* of a data point $\mathbf{x}$ is the Euclidean distance between $\mathbf{x}$ and its reconstructed data point $\tilde{\mathbf{x}}$, where $\tilde{\mathbf{x}}$ is the representation of $\mathbf{x}$ in terms of the principal components.

PCA

No, it will not decrease the reconstruction error, which was already 0 from part (b).

Neural Networks

Question: Suppose we have a neural network for performing nonlinear regression which consists of three linear layers, where all but the last layer have a sigmoid activation and the last layer uses a linear activation. Letting $\mathbf{x}_0 \in \mathbb{R}^{d_0}$ denote the d_0-dimensional input to the network and $\hat{y}$ the scalar output, we can write

$$\begin{aligned} \mathbf{x}_1 &= A_1\mathbf{x}_0 + b_1\mathbf{1}, \quad \tilde{\mathbf{x}}_1 = \sigma(\mathbf{x}_1) \\ \mathbf{x}_2 &= A_2\tilde{\mathbf{x}}_1 + b_2\mathbf{1}, \quad \tilde{\mathbf{x}}_2 = \sigma(\mathbf{x}_2) \\ \hat{y} = x_3 &= A_3\tilde{\mathbf{x}}_2 + b_3. \end{aligned}$$

Here our model parameters are the bias terms $b_1, b_2, b_3 \in \mathbb{R}$ and the matrices $A_1 \in \mathbb{R}^{d_1 \times d_0}, A_2 \in \mathbb{R}^{d_2 \times d_1}, A_3 \in \mathbb{R}^{1 \times d_2}$, where the hidden states $\mathbf{x}_1 \in \mathbb{R}^{d_1}$ and $\mathbf{x}_2 \in \mathbb{R}^{d_2}$. Normally, we optimize the parameters of our neural network $A_1, A_2, A_3, b_1, b_2, b_3$ in order to minimize a given loss function. Now, suppose we are instead trying to attack the neural network in order to cause it to obtain the *wrong* answer by choosing the input $\mathbf{x}_0$ that *maximizes* the loss.

Question: Suppose we use the l_2 loss function $\mathcal{L}(\hat{y}, y^*) = ||\hat{y} - y^*||_2^2$, where y^* is the ground truth label. Express $\frac{\partial \mathcal{L}}{\partial \mathbf{x}_0}$ in terms of y^*, parameters $A_1, A_2, A_3, b_1, b_2, b_3$, and intermediate values $\mathbf{x}_0, \mathbf{x}_1, \mathbf{x}_2, x_3, \tilde{\mathbf{x}}_1, \tilde{\mathbf{x}}_2$.

$$\frac{\partial \mathcal{L}}{\partial x_3} = \frac{\partial}{\partial \hat{y}}(x_3 - y^*)(x_3 - y^*) = 2(x_3 - y^*)$$
$$\frac{\partial \mathbf{x}_i}{\partial \tilde{\mathbf{x}}_{i-1}} = \frac{\partial}{\partial \tilde{\mathbf{x}}_{i-1}}(A_i \tilde{\mathbf{x}}_{i-1} + b_i) = A_i$$
$$\frac{\partial \tilde{\mathbf{x}}_i}{\partial \mathbf{x}_i} = \frac{\partial}{\partial \mathbf{x}_i}\sigma(\mathbf{x}_i) = \text{diag}(\sigma(\mathbf{x}_i)(1 - \sigma(\mathbf{x}_i)))$$

$$\frac{\partial \mathcal{L}}{\partial \mathbf{x}_0} = \frac{\partial \mathcal{L}}{\partial x_3}\frac{\partial x_3}{\partial \tilde{\mathbf{x}}_2}\frac{\partial \tilde{\mathbf{x}}_2}{\partial \mathbf{x}_2}\frac{\partial \mathbf{x}_2}{\partial \tilde{\mathbf{x}}_1}\frac{\partial \tilde{\mathbf{x}}_1}{\partial \mathbf{x}_1}\frac{\partial \mathbf{x}_1}{\partial \mathbf{x}_0}$$
$$= 2(x_3 - y^*)A_3\text{diag}(\sigma(\mathbf{x}_2)(1 - \sigma(\mathbf{x}_2)))A_2\text{diag}(\sigma(\mathbf{x}_1)(1 - \sigma(\mathbf{x}_1)))A_1$$

Question: Use your answer to part (a) to write the expression for a gradient update with a learning rate of λ for $\mathbf{x}_0$ that will *maximize* the loss $\mathcal{L}(\hat{y}, y^*) = ||\hat{y} - y^*||_2^2$ when performed repeatedly.

Normally, we perform gradient *descent* by subtracting the learning rate times the gradient. In this case, we are trying to maximize the loss, so must instead perform gradient *ascent*:

$$\mathbf{x}_0 \leftarrow \mathbf{x}_0 + \lambda \frac{\partial \mathcal{L}}{\partial \mathbf{x}_0}$$

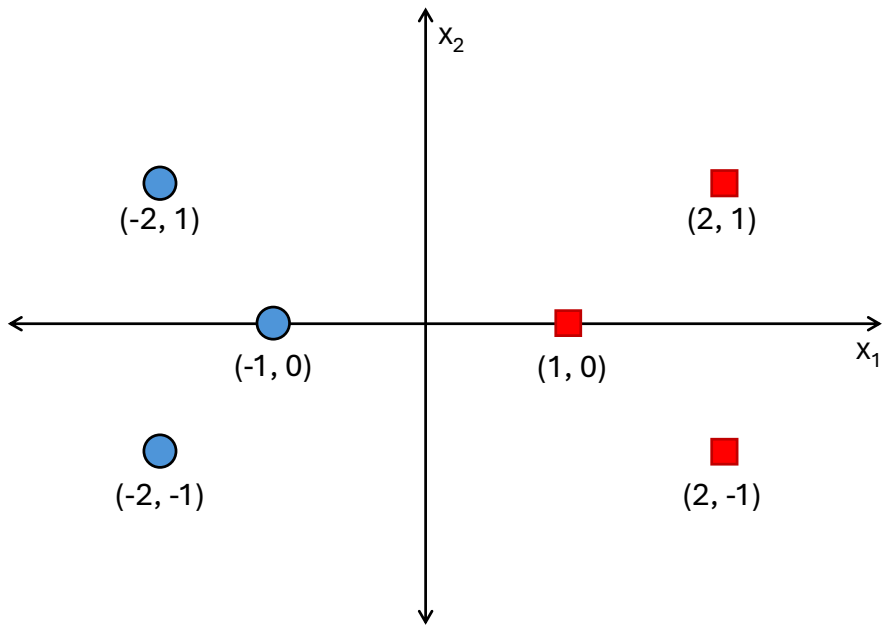
Question: Assuming a constant learning rate that is appropriately small, is the loss value associated with the gradient-based optimization procedure you described in part (b) guaranteed to converge? Why or why not?

The loss is not guaranteed to converge. Normally, we optimize a loss metric which is bounded in the direction of optimization, e.g. minimizing the l_2 error with the constraint that the l_2 error cannot be negative. So long as the loss decreases monotonically, this guarantees convergence eventually.

However, in this case, the l_2 loss is not bounded above. As such, it can, if not constrained in some way, diverge to $+\infty$. This is commonly done by restricting $||x' - x||_p < \varepsilon$ for some p-norm and distance ε; once the gradient ascent algorithm above is modified to take this into account, this results in a procedure commonly known as *projected gradient descent*.

Ensemble Methods

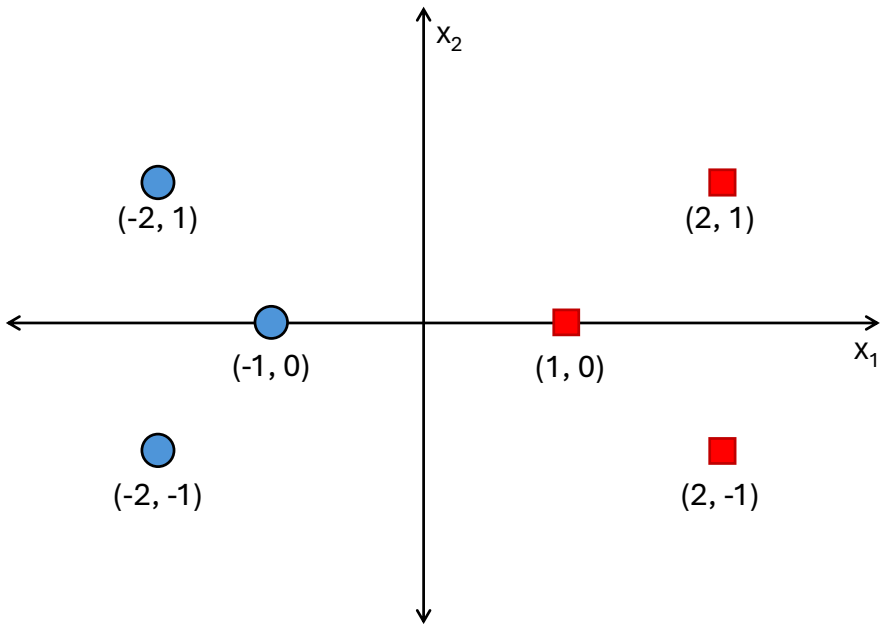
Question: Recall that ensemble methods aim to train multiple decision trees and combine their results to produce a classifier. In this problem, we will apply ensemble methods to the dataset of six points shown in the figure below. Each dataset has a two-dimensional input $\begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$, with coordinates shown as (x_1, x_2) in the figure. Each data point's label is indicated by a blue circle or red square.



Question: First, we apply random forests to this dataset. We use $n = 2$ data points for each tree and train $m = 5$ trees. Find an expression for the probability that $\mathbf{x} = \begin{bmatrix} 2 \\ 1 \end{bmatrix}$ is used to train the fifth tree. You may assume that data points are sampled with replacement. If it is not possible to derive this probability without knowledge of the first four trees, explain why not.

Each data point has an equal probability of being chosen to train each tree in the ensemble. We choose $n = 2$ out of $N = 6$ data points with replacement, so the probability of being chosen is $1 - \left(\frac{N-1}{N}\right)^n = 1 - \left(\frac{5}{6}\right)^2 = \frac{11}{36}$.

Question: Now suppose that you try AdaBoost on this dataset, and you decide to use decision stumps (one-layer decision trees) as your base classifiers. Find the first decision stump that is created by AdaBoost. You can provide your answer by drawing the line in the figure below, or by providing the equation of the decision boundary.



Any vertical line $x_1 = \alpha$ for $\alpha \in (-1, 1)$ is correct.

Question: Continuing from the decision stump found in part (b), you decide to run AdaBoost for four more iterations, so that your final ensemble has five decision stumps. Find the probability that the data point $\begin{bmatrix} 2 \\ 1 \end{bmatrix}$ has higher weight than the data point $\begin{bmatrix} -2 \\ 1 \end{bmatrix}$ in training the fifth decision stump in AdaBoost.

Both data points will have equal weight for all classifiers in the ensemble, since from part (b) the first classifier has zero training error.

In general, this statement may not be true, as the weight of each data point $\mathbf{x}$ depends on the value $h_t(\mathbf{x})$ of each base classifier. However, since we are using decision stumps, the base classifier value is binary, so each correctly classified data point has the same classifier value $h_t(\mathbf{x})$.

Ensemble Methods

Question: How many data points in this dataset will be misclassified by the resulting ensemble of five trees from part (c)? Explain your answer or show your work.

All data points will be correctly classified. Since all points are correctly classified by the first tree, all subsequent trees will also correctly classify each data point.

Ensemble Methods

Question: Considering again the ensemble learned in part (c), will the misclassification rate on a test dataset be larger or smaller than the misclassification rate on the training dataset? Briefly explain your answer. If it is not possible to know the answer without information on the testing dataset, explain why not.

Since the misclassification rate on the training dataset is zero, the misclassification rate on the test dataset must be either equal to or larger than the rate on the training dataset.