ECE M146 Homework 8 Solution
Introduction to Machine Learning
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Please upload your homework to Gradescope by June 8, 11:59 pm.
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1. In class, you learned that the direction that maximizes the variance of the projection onto a one-dimensional space is the eigenvector corresponds to the largest eigenvalue of the data covariance matrix $S = \frac{1}{N}X^TX$, where $X = \begin{bmatrix} x_1^T - \bar{x}^T \\ \cdots \\ x_n^T - \bar{x}^T \end{bmatrix}$. Formally, the solution to the following maximization problem

$$\max_{u_1} u_1^T S u_1 \quad \text{subject to } \|u_1\|^2 = 1,$$

is the eigenvector corresponds to the largest eigenvalue of S.

In this exercise, we use proof by induction to show that the linear projection onto an M-dimensional subspace that maximizes the variance of the projected data is defined by the M eigenvectors of the data covariance matrix S corresponding to the M largest eigenvalues. Now suppose the result holds for some general value of M and show that it consequently holds for dimensionality $M+1$. To do this, first set the derivative of the variance of the projected data with respect to a vector u_{M+1} defining the new direction in data space equal to zero. This should be done subject to the constraints that u_{M+1} be orthogonal to the existing vectors $u_1, \cdots, u_M$, and also that it be normalized to unit length. Use Lagrange multipliers to enforce these constraints. Then make use of the orthonormality properties of the vectors $u_1, \cdots, u_M$ to show that the new vector u_{M+1} is an eigenvector of S. Finally, show that the variance, i.e., $u_{M+1}^T S u_{M+1}$, is maximized if we choose u_{M+1} to be the eigenvector that corresponds to the $M+1$-st largest eigenvalue λ_{M+1}, assuming the eigenvalues have been ordered in decreasing value.
Solution: We use a Lagrange multiplier λ_{M+1} to enforce the unit norm constraint $u_{M+1}^T u_{M+1} = 1$. We use Lagrange multipliers $\eta_1, \cdots, \eta_M$ to enforce the constraints that u_{M+1} is orthogonal to $u_1, \cdots, u_M$. The Lagrangian is then:

$$L(u_{M+1}, \lambda_{M+1}, \eta_{1,\cdots,M}) = u_{M+1}^T S u_{M+1} + \lambda_{M+1}(1 - u_{M+1}^T u_{M+1}) + \sum_{i=1}^{M} \eta_i u_{M+1}^T u_i).$$

Setting $\nabla_{u_{M+1}} L(u_{M+1}, \lambda_{M+1}, \eta_{1,\cdots,M}) = 0$, we get

$$0 = 2Su_{M+1} - 2\lambda_{M+1}u_{M+1} + \sum_{i=1}^{M} \eta_i u_i.$$

Left multiplying with u_j^T and using the orthogonality constraints, we see that $\eta_j = 0$ for $j = 1, \cdots, M$. We therefore obtain

$$Su_{M+1} = \lambda_{M+1} u_{M+1}.$$

This shows that the new vector u_{M+1} is an eigenvector of S. Left multiply both sides with u_{M+1} and use the normalization constraint, we have

$$\lambda_{M+1} = u_{M+1}^T S u_{M+1}.$$

Then the eigenvector should be the one that corresponds to the $M + 1$-st largest eigenvalue.

2. Suppose you have four data points: $x_1 = [2, 2, 0]^T, x_2 = [0, -2, 2]^T, x_3 = [-2, 0, 0]^T$ and $x_4 = [0, 0, -2]^T$. Use what you learned in PCA to find the 2-dimensional projection of these data points that maximize the sum variance. You should be able to solve this question by hand.

Solution: The data have a mean of $[0, 0, 0]^T$. We first calculate the data covariance matrix:

$$S = \frac{1}{4}\left[\begin{bmatrix} 4 & 4 & 0 \\ 4 & 4 & 0 \\ 0 & 0 & 0 \end{bmatrix} + \begin{bmatrix} 0 & 0 & 0 \\ 0 & 4 & -4 \\ 0 & -4 & 4 \end{bmatrix} + \begin{bmatrix} 4 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} + \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 4 \end{bmatrix}\right] = \begin{bmatrix} 2 & 1 & 0 \\ 1 & 2 & -1 \\ 0 & -1 & 2 \end{bmatrix}.$$

We next find the eigenvalues of S to be $2 + \sqrt{2}, 2$ and $2 - \sqrt{2}$ with eigenvectors $[-0.5, -\frac{\sqrt{2}}{2}, 0.5]^T$, $[\frac{\sqrt{2}}{2}, 0, \frac{\sqrt{2}}{2}]^T$ and $[-0.5, \frac{\sqrt{2}}{2}, 0.5]^T$, respectively.

We choose the eigenvectors that correspond to the largest 2 eigenvalues to be the subspace we wish to project on. Define s_i to be projected data for x_i. The transformation for x_i can then be written as:

$$s_i = \begin{bmatrix} -0.5 & -\frac{\sqrt{2}}{2} & 0.5 \\ \frac{\sqrt{2}}{2} & 0 & \frac{\sqrt{2}}{2} \end{bmatrix} x_i.$$

We finally get

$$s_1 = \begin{bmatrix} -1 - \sqrt{2} \\ \sqrt{2} \end{bmatrix}, s_2 = \begin{bmatrix} 1 + \sqrt{2} \\ \sqrt{2} \end{bmatrix}, s_3 = \begin{bmatrix} 1 \\ -\sqrt{2} \end{bmatrix}, \text{and } s_4 = \begin{bmatrix} -1 \\ -\sqrt{2} \end{bmatrix}.$$

3. One application of PCA is compression. Suppose we want to compress a data vector $x_n \in \mathbf{R}^D$ into M dimensions. We can write the PCA approximation to a data vector x_n in the form:

$$\tilde{x}_n = \sum_{i=1}^{M} (x_n^T u_i) u_i + \sum_{i=M+1}^{D} (\bar{x}^T u_i) u_i$$
$$= \bar{x} + \sum_{i=1}^{M} (x_n^T u_i - \bar{x}^T u_i) u_i,$$

where $\bar{x}$ is the mean vector of $\{x_1, \cdots, x_N\}$ and $\{u_1, \cdots, u_D\}$ are the eigenvectors (corresponding to the largest to smallest eigenvalues) of the data covariance matrix:

$$S = \frac{1}{N} \sum_{i=1}^{N} (x_i - \bar{x})(x_i - \bar{x})^T.$$

In this exercise, you are given part of the MNIST dataset that has handwritten 4 in it. The data is in the file *MNIST4.csv* which contains a matrix of size 400×784. Each row of the matrix represent an image of size 28×28 where each element represents the intensity of each pixel in gray scale. The 400 images are shown in Figure 1.

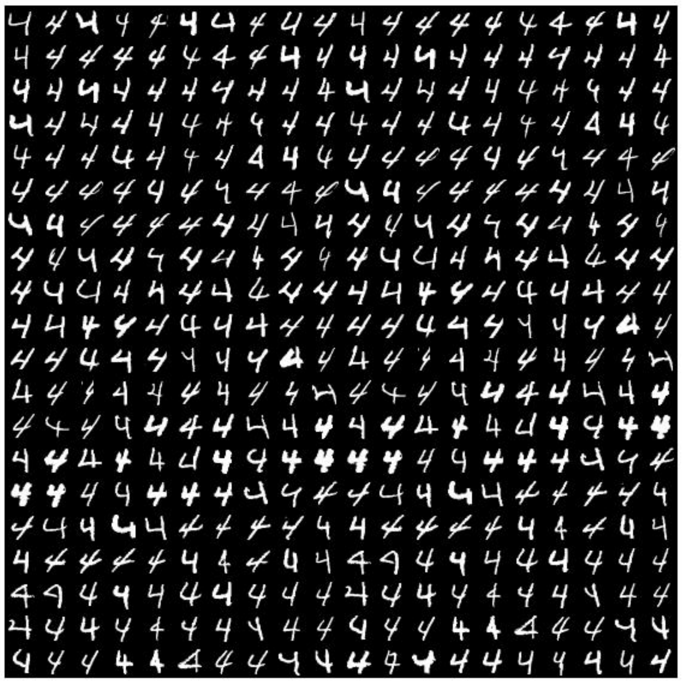
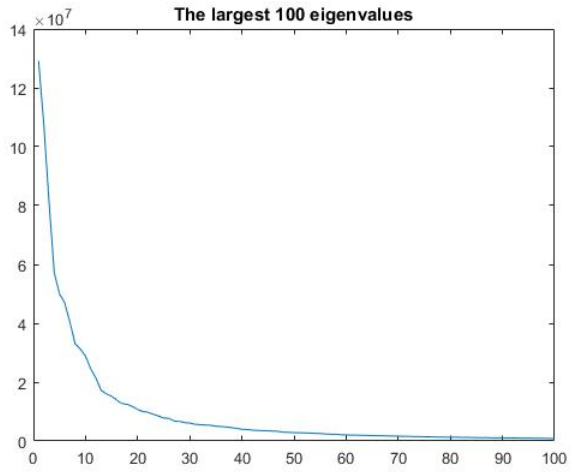


Figure 1: 400 images of 4

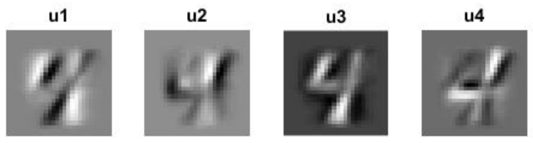
(a) **Eigenvalues** Calculate the eigenvalues and eigenvectors of the data covariance matrix. You may use `eig` in MATLAB and `scipy.linalg.eigh` in Python. Do not use `numpy.linalg.eig` as it will give complex eigenvalues. Plot the 100 largest eigenvalues.

Solution:



(b) **Eigenvectors visualization** Visualize the first 4 eigenvectors by first reshaping the eigenvector into size 28×28 and then showing it as an image using *imshow*. For a better visualization result, scale the range of each eigenvector into $[0-255]$. What do you observe?

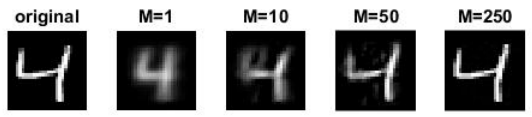
Solution:



The 4 largest eigenvectors have the shape 4 in it. Some difference due to complex eigenvalues are okay.

(c) **Compression using PCA** Compress the first image, i.e., the one on the top left corner, into $M = 1, 10, 50$ and 250 dimensions. Plot the compressed images along with the original image in the same figure. Note that the original image corresponds to $M = 784$. Comment on the quality of the compressed images. What do you get when $M = 0$?

Solution:



The image quality gets better with large M. We notice that the image quality is already pretty good with $M = 15$ and 50. When $M = 0$, the compressed image is just the mean image of the 400 images. Please grade based on the relative quality of the images. For $M = 250$, the result may be different for python user if you use `numpy.linalg.eig`.

4. In this question, we are going to derive results that give us intuition about bagging. Suppose we have N balls in a jar that are numbered $1, \cdots, N$.

   (a) We pick the ball randomly one at a time without replacement. What is the probability that ball 1 is not picked in N realization of this experiment?
   Solution: This probability is 0. Out of the N balls we picked, one ball must be ball 1 because we pick without replacement.

   (b) We pick the ball randomly one at a time with replacement. What is the probability that ball 1 is not picked in N realization of this experiment?
   Solution: $P = \left(1 - \frac{1}{N}\right)^N$.

   (c) For $N = 1000$, verify that the expression you get in (b) is close to $1/e = 0.3679$. Show that probability you get in (b) approaches $\frac{1}{e}$ when $N \to \infty$. Hint: Take the natural log of the limit and then apply the L'Hospital's Rule.
   Solution: We are trying to find the following limit:

$$a = \lim_{N\to\infty} \left(1 - \frac{1}{n}\right)^N .$$

   Taking natural log of this limit, we get

$$\begin{aligned}
\ln a &= \lim_{N\to\infty} N \ln(1 - \frac{1}{N}) \\
&= \lim_{N\to\infty} \frac{\ln(1 - \frac{1}{N})}{\frac{1}{N}} \\
&= \lim_{N\to\infty} \frac{\frac{1}{1-\frac{1}{N}} \cdot \left(\frac{1}{N}\right)^2}{-\left(\frac{1}{N}\right)^2} \\
&= \lim_{N\to\infty} -\frac{1}{1 - \frac{1}{N}} \\
&= -1.
\end{aligned}$$

   We then get $a = \frac{1}{e}$.

5. In class, we learned that the log likelihood function for the Gaussian mixture model is of this form:

$$J = \ln P(X|\pi, \mu, \Sigma) = \sum_{n=1}^{N} \ln \left\{ \sum_{k=1}^{K} \pi_k \mathcal{N}(x_n|\mu_k, \Sigma_k) \right\}.$$

Here, π_k is the prior probability of each Gaussian component; μ_k and Σ_k are the mean and covariance matrix for the k-th Gaussian component.

Suppose we want to maximize J with respect to π_k. Here we must take account of the constraint $\sum_{k=1}^{K} \pi_k = 1$. Use a Lagrange multiplier to enforce this constraint. Show that the π_k that maximize J is of the form:

$$\pi_k = \frac{N_k}{N},$$

where

$$N_k = \sum_{n=1}^{N} \gamma(z_{nk}),$$

and

$$\gamma(z_{nk}) = \frac{\pi_k \mathcal{N}(x_n|\mu_k, \Sigma_k)}{\sum_{j=1}^{K} \pi_j \mathcal{N}(x_n|\mu_j, \Sigma_j)}.$$

You may assume that all $\gamma(z_{nk})$ are known for this step.
Solution: Using a Lagrange multiplier, we maximize the following quantity

$$\ln P(X|\pi, \mu, \Sigma) + \lambda \left(\sum_{k=1}^{K} \pi_k - 1 \right).$$

Taking derivative with respect to π_k and set it equals 0 gives:

$$0 = \sum_{n=1}^{N} \frac{\mathcal{N}(x_n|\mu_k, \Sigma_k)}{\sum_{j=1}^{K} \pi_j \mathcal{N}(x_n|\mu_j, \Sigma_j)} + \lambda. \tag{1}$$

Multiply both side by π_k and sum over all k. We get

$$0 = \sum_{k=1}^{N} \sum_{n=1}^{N} \frac{\pi_k \mathcal{N}(x_n|\mu_k, \Sigma_k)}{\sum_{j=1}^{K} \pi_j \mathcal{N}(x_n|\mu_j, \Sigma_j)} + \lambda \sum_{k=1}^{K} \pi_k.$$

Make use of the constraint $\sum_{k=1}^{K} \pi_k = 1$. We get

$$\lambda = -N.$$

Multiply (1) both side with π_k and substitute λ and the definition of N_k. We find

$$\pi_k = \frac{N_k}{N}.$$

6. In this exercise, you will implement the algorithm on page 167 of *A course in Machine Learning* and use it to perform classification on the data in *AdaBoost_data.csv.*

   (a) **Visualization** The data file contains a matrix in which the 11 rows represent 11 data points. For each row, the first two columns contain the values of x_1 and x_2 and the third column contains the label y for each data point.

   Generate a scatter plot of the dataset where data points from different classes are plotted using different color. Is this dataset linearly separable? Can we use a single layer decision tree to classify all points correctly?

   Solution: Plot is in the figure for $k = 1$ below. The data is not linearly separable. It can not be classified all correctly using a single layer decision tree.

   (b) **Implementation** Consider the decision stump (1 layered decision tree) of the following form as the base classifier for the AdaBoost algorithm.

$$\hat{y} = \text{sign}(s(x_i - t)), s \in \{+1, -1\}, i \in \{1, 2\}, t \in \mathbb{Z}.$$

   The above classifier simply classifies x_i to the right of the threshold t as either $+1$ or -1 based on the sign of either $x_i - t$ or $t - x_i$. For simplicity, in this problem, we restrict t to be integer. The data is designed to avoid the evaluation of sign(0).

   Implement the AdaBoost algorithm on page 167 of *A course in Machine Learning* using the above base classifier for $K = 3$. Use natural log for the log operator in the algorithm and make sure to normalize the weights so that all weights sum to 1. To train the k-th classifier, for $i \in \{1, 2\}$ and $s \in \{+1, -1\}$, search through all integers in the range of x_i exhaustively and find $t^{(k)}$ that minimizes the weighted misclassification error $\hat{\epsilon}^{(k)}$. To avoid exhaustive search for both s and i, we provide the optimal s and i for each iteration as follows: for $k = 1, i = 1, s = -1$; for $k = 2, i = 1, s = -1$; for $k = 3, i = 2, s = 1$. Choose the smaller t in the case that multiple t's give the same weighted misclassification error.

   As a sanity check, you should get $t^{(1)} = 3$ which gives you the first decision stump as:

$$\hat{y} = \text{sign}(3 - x_1).$$

   Run the algorithm and report $d^{(0)}$,$d^{(1)}$ and $d^{(2)}$ in a table. What is your $t^{(k)}$ and $\alpha^{(k)}$ for $k = 1, 2$ and 3? What is the final combined classifier? What is the training accuracy using this combined classifier?

   Plot the data as a scatter plot for $k = 1, 2$ and 3 with the size of each point proportional to $d^{(k-1)}$. Draw the decision boundary of each decision stump.

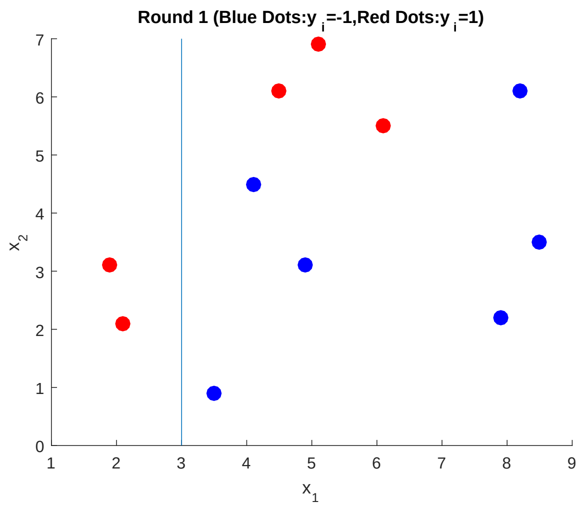
   Solution: The weights are reported in the following table. We get $t^{(1)} = 3$, $t^{(2)} = 7$, $t^{(3)} = 5$, $a^{(1)} = 0.4904$, $a^{(2)} = 0.7332$ and $a^{(3)} = 1.0184$. As a result, the final classifier is:

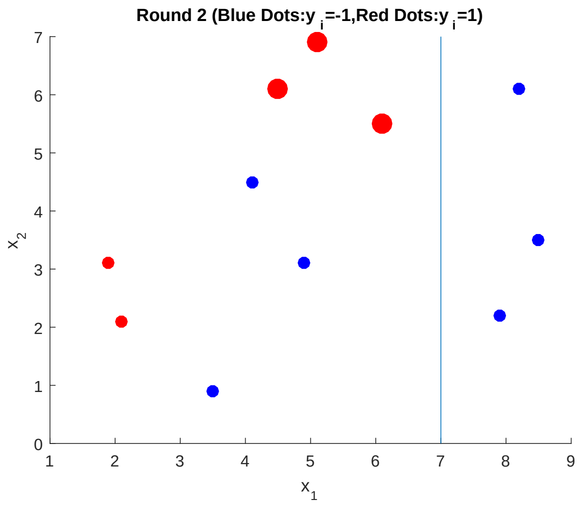
$$\hat{y} = \text{sign}[0.4904 \times \text{sign}(3 - x_1) + 0.7332 \times \text{sign}(7 - x_1) + 1.0184 \times \text{sign}(x_2 - 5)].$$

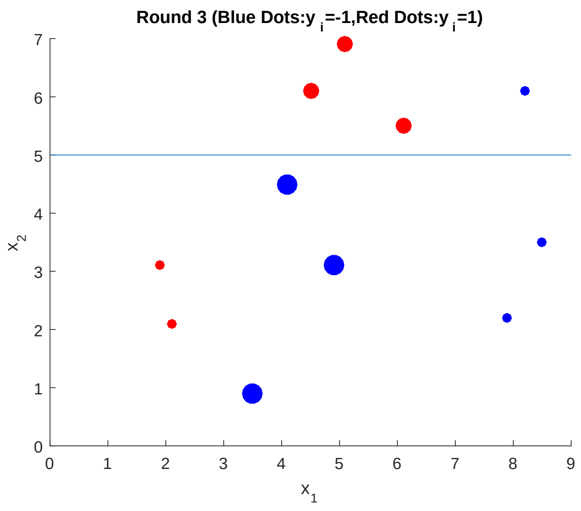
   This classifier classifies all training points correctly.

   The plots are shown in the subsequent figures.

data #	$d^{(0)}$	$d^{(1)}$	$d^{(2)}$
1	0.0909	0.0625	0.0385
2	0.0909	0.0625	0.0385
3	0.0909	0.1667	0.1026
4	0.0909	0.0625	0.1667
5	0.0909	0.0625	0.1667
6	0.0909	0.1667	0.1026
7	0.0909	0.0625	0.1667
8	0.0909	0.1667	0.1026
9	0.0909	0.0625	0.0385
10	0.0909	0.0625	0.0385
11	0.0909	0.0625	0.0385




Round 2 (Blue Dots:y_i=-1,Red Dots:y_i=1)
x_1
x_2
0 1 2 3 4 5 6 7
1 2 3 4 5 6 7 8 9


Round 3 (Blue Dots:y_i=-1,Red Dots:y_i=1)
x_1
x_2
0
1
2
3
4
5
6
7
8
9