Boston University
Department of Electrical and Computer Engineering

ENG EC 414 Introduction to Machine Learning

HW 9 Solution

Issued: Fri 13 Nov 2020 **Due:** 10:00am Fri 19 Nov 2020 in Gradescope

Important: Before you proceed, please read the documents pertaining to *Homework formatting and submission guidelines* in the Homeworks section of Blackboard. **In particular, for computer assignments you are prohibited from using any online code or built-in MATLAB functions except as indicated in the problem or skeleton code (when provided).**

Important: To obtain full grade, please clearly motivate all your answers.

Note: Problem difficulty = number of coffee cups ☕

Problem 9.1 [15pts] *(PCA by hand)*

(a) [5pts] Let $\mathrm{S} = \begin{bmatrix} a & 0 \\ 0 & b \end{bmatrix}$. Verify that this matrix has two eigenvalues, a and b, and that the corresponding eigenvectors are $\mathbf{u}_1 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$ and $\mathbf{u}_2 = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$

(b) [5pts] Consider the following data points:

$$\mathbf{x}_1 = \begin{bmatrix} 1 \\ 3 \end{bmatrix}, \mathbf{x}_2 = \begin{bmatrix} 1 \\ 7 \end{bmatrix}, \mathbf{x}_3 = \begin{bmatrix} 0 \\ 5 \end{bmatrix}, \mathbf{x}_4 = \begin{bmatrix} 2 \\ 5 \end{bmatrix},$$

Compute the empirical covariance matrix of the above four data points, that is, $\frac{1}{4}\sum_{i=1}^{4}(\mathbf{x}_i - \hat{\boldsymbol{\mu}}_x)\cdot(\mathbf{x}_i - \hat{\boldsymbol{\mu}}_x)^\top$ where $\hat{\boldsymbol{\mu}}_x$ is the empirical mean vector of the data points.

(c) [5pts] Compute the eigenvector of the covariance matrix from part (b) corresponding to the largest eigenvalue (this is the first principal direction) and the corresponding principal components of the four data points along this direction.

Solution:

(a) [5pts] Since $\mathbf{u}_1$ and $\mathbf{u}_2$ are both non-zero vectors, we only need to verify that $\mathrm{S}\mathbf{u}_1 = a\mathbf{u}_1$ and $\mathrm{S}\mathbf{u}_2 = a\mathbf{u}_2$ to establish that $\mathbf{u}_1$ and $\mathbf{u}_2$ are indeed eigenvectors of S with eigenvalues a and b respectively:

$$\mathrm{S}\mathbf{u}_1 = \begin{bmatrix} a & 0 \\ 0 & b \end{bmatrix}\begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} a \\ 0 \end{bmatrix} = a\begin{bmatrix} 1 \\ 0 \end{bmatrix} = a\,\mathbf{u}_1, \quad \mathrm{S}\mathbf{u}_2 = \begin{bmatrix} a & 0 \\ 0 & b \end{bmatrix}\begin{bmatrix} 0 \\ 1 \end{bmatrix} = \begin{bmatrix} 0 \\ b \end{bmatrix} = b\begin{bmatrix} 0 \\ 1 \end{bmatrix} = b\,\mathbf{u}_2$$

(b) [5pts] The empirical mean vector $\hat{\boldsymbol{\mu}}_x$ is equal to

$$\hat{\boldsymbol{\mu}}_x = \frac{1}{4}\sum_{j=1}^{4}\mathbf{x}_j = \frac{1}{4}\left\{\begin{bmatrix} 1 \\ 3 \end{bmatrix} + \begin{bmatrix} 1 \\ 7 \end{bmatrix} + \begin{bmatrix} 0 \\ 5 \end{bmatrix} + \begin{bmatrix} 2 \\ 5 \end{bmatrix}\right\} = \frac{1}{4}\begin{bmatrix} 4 \\ 20 \end{bmatrix} = \begin{bmatrix} 1 \\ 5 \end{bmatrix}$$

The empirical covariance matrix of this dataset is equal to:

$$
\begin{aligned}
\hat{\mathrm{S}}_x &= \frac{1}{4}\sum_{j=1}^{4}(\mathbf{x}_j - \hat{\boldsymbol{\mu}}_x)\cdot(\mathbf{x}_j - \hat{\boldsymbol{\mu}}_x)^\top = \left(\frac{1}{4}\sum_{j=1}^{4}\mathbf{x}_j\mathbf{x}_j^\top\right) - \hat{\boldsymbol{\mu}}_x\hat{\boldsymbol{\mu}}_x^\top \\
&= \frac{1}{4}\left\{\begin{bmatrix}1\\3\end{bmatrix}\cdot\begin{bmatrix}1 & 3\end{bmatrix} + \begin{bmatrix}1\\7\end{bmatrix}\cdot\begin{bmatrix}1 & 7\end{bmatrix} + \begin{bmatrix}0\\5\end{bmatrix}\cdot\begin{bmatrix}0 & 5\end{bmatrix} + \begin{bmatrix}2\\5\end{bmatrix}\cdot\begin{bmatrix}2 & 5\end{bmatrix}\right\} - \begin{bmatrix}1\\5\end{bmatrix}\cdot\begin{bmatrix}1 & 5\end{bmatrix} \\
&= \frac{1}{4}\left\{\begin{bmatrix}1 & 3\\3 & 9\end{bmatrix} + \begin{bmatrix}1 & 7\\7 & 49\end{bmatrix} + \begin{bmatrix}0 & 0\\0 & 25\end{bmatrix} + \begin{bmatrix}4 & 10\\10 & 25\end{bmatrix}\right\} - \begin{bmatrix}1 & 5\\5 & 25\end{bmatrix} \\
&= \frac{1}{4}\begin{bmatrix}6 & 20\\20 & 108\end{bmatrix} - \begin{bmatrix}1 & 5\\5 & 25\end{bmatrix} \\
&= \begin{bmatrix}1^1/_2 & 5\\5 & 27\end{bmatrix} - \begin{bmatrix}1 & 5\\5 & 25\end{bmatrix} \\
&= \begin{bmatrix}^1/_2 & 0\\0 & 2\end{bmatrix}
\end{aligned}
$$

(c) [5pts] From part (a), the eigenvalues of $\hat{\mathrm{S}}_x$ are $a = \frac{1}{2}$ and $b = 2$ and correspond to eigenvectors $\mathbf{u}_1$ and $\mathbf{u}_2$ respectively. Since the largest eigenvalue is 2, the first principal direction is $\mathbf{u}_2$. The principal components of the four data points along $\mathbf{u}_2$ are given by their projections onto $\mathbf{u}_2$ after centering:

$$
\begin{aligned}
\mathbf{u}_2^\top(\mathbf{x}_1 - \hat{\boldsymbol{\mu}}_x) &= 3 - 5 = -2, \\
\mathbf{u}_2^\top(\mathbf{x}_2 - \hat{\boldsymbol{\mu}}_x) &= 7 - 5 = 2, \\
\mathbf{u}_2^\top(\mathbf{x}_3 - \hat{\boldsymbol{\mu}}_x) &= 5 - 5 = 0, \\
\mathbf{u}_2^\top(\mathbf{x}_4 - \hat{\boldsymbol{\mu}}_x) &= 5 - 5 = 0.
\end{aligned}
$$

Thus the (first) principal components of the four points along $\mathbf{u}_2$ are $\{-2, 2, 0, 0\}$.

Problem 9.2 [34pts] *(PCA of Images)* In this problem we will perform Principal Component Analysis (PCA) on the AT&T Face Dataset. We provided a skeleton code, but you don't have to submit any code for this problem, just figures and results.

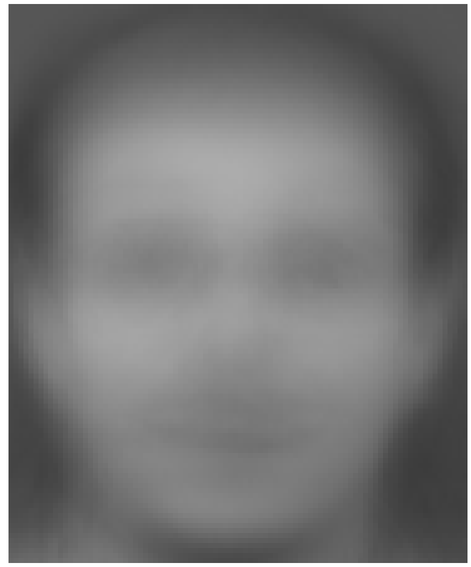
AT&T Face Dataset: This dataset contains 400 images (10 images of 40 diffferent people) of size 112×92 (10304 pixels) in the Portable Grayscale Map (PGM) format. We have provided you this dataset as `att-database-of-faces.zip` and a helper function `load_faces.m` to load the dataset into your MATLAB workspace as a matrix of "vectorized" images of dimensions 400×10304. Unzip the dataset and place the resulting folder named `att-database-of-faces` in the same directory as your solution file to use `load_faces.m`.

Tasks:

(a) [5pts] *(Data Visualization)* Use the provided `load_faces.m` function and load the face-dataset into your workspace. Compute the mean face image, that is the mean of all the 400 face image vectors. Use `subplot` and `imshow(uint8(reshape(img_vector, img_size)))` to create a figure containing two images: (1) image #120 in the dataset, and (2) the mean face of the dataset. Does the mean face resemble a human face or is it a smooth shapeless "blob"?

Solution: Image #120 and the mean of all faces in the AT&T Face Dataset are shown in Figure 1. The mean face looks extremely blurred, but key facial features such as the eyes, nose, mouth, ears, hair and outline of face are still recognizable.

(1)



(2)

Figure 1: ***Problem 9.2(a):*** ***(1)*** *Image #120 in AT&T Face Dataset.* ***(2)*** *The mean of all faces in the AT&T Face Dataset.*

(b) [20pts] *(Eigenvalues of Covariance Matrix)* Subtract the vectorized mean face image $\hat{\boldsymbol{\mu}}_x$ from all the vectorized face images and compute the empirical covariance matrix $\hat{\mathrm{S}}_x$ of the mean-centered vectorized face images. Perform an Eigenvalue Decomposition of this covariance matrix using the inbuilt MATLAB fucntion `eig`. Arrange the eigenvectors $\mathbf{u}_1, \mathbf{u}_2, \ldots$ in the order of non-increasing eigenvalues $\lambda_1 \geq \lambda_2 \geq \ldots$, into an orthonormal matrix $U = [\mathbf{u}_1, \mathbf{u}_2, \ldots]$. Let Λ be the corresponding diagonal matrix of eigenvalues.

(1) [5pts] Report the values of the first five eigenvalues.

(2) [5pts] Plot λ_k as a function of k, for $k = 1, 2, \ldots, 450$. Comment on the observed trends in your report. Explain why $\lambda_k = 0$ for all $k > 400$.

(3) [5pts] Compute and plot (as a function of k) the values of the so-called "fraction of variance explained" by the top k principal components:

$$\rho_k := \frac{\sum_{i=1}^{k} \lambda_i}{\sum_{i=1}^{d} \lambda_i}.$$

Round the values of ρ_k to 2 decimal places. Comment on the observed trends in your report.

(4) [5pts] Find and report the smallest values of k for which $\rho_k \geq 0.51, 0.75, 0.90, 0.95$, and 0.99.

Notes: Use subplots to show plots of λ_k and ρ_k in the same figure. The reshaped principal directions of a human face dataset are often referred to as eigenfaces.

Solution: (1) [5pts] The top five eigenvalues are $\lambda_1 = 2,823,900$, $\lambda_2 = 2,069,700$, $\lambda_3 = 1,097,000$, $\lambda_4 = 894,700$, $\lambda_5 = 819,400$.

(2) [5pts] The plots of λ_k and $\ln(\lambda_k)$ as functions of k are shown in Figure 2(i) and (ii). The value of λ_k (and therefore also $\ln(\lambda_k)$)) decrease as k increases since the eigenvalues have been sorted in

a non-increasing order. There is, however, no clear knee or elbow at which there is a clear bend. The curves keep decreasing very smoothly. Yet, roughly speaking, we could say that by $k = 100$ or so the curves have essentially plateaued-out. Moreover, all eigenvalues beyond $k = 400$ are exactly zero. This is because there are only $n = 400$ images in this dataset. Hence the empirical covariance matrix cannot have a rank r which greater than n. Hence all eigenvalues beyond $k = r$ are zero, i.e., $\lambda_{r+1} = \ldots = \lambda_d = 0$, where $d = 10,304$.

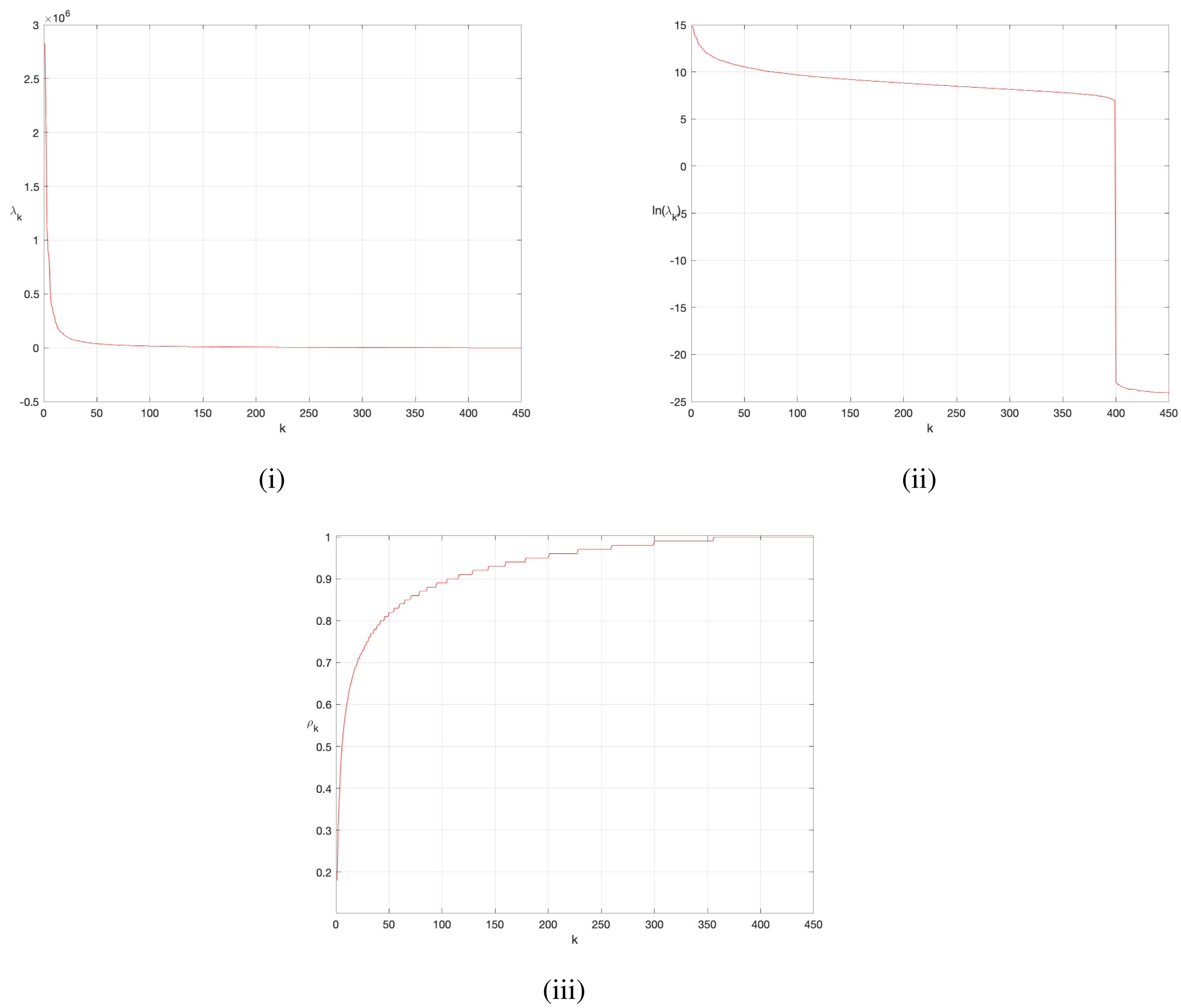


Figure 2: ***Problem 9.2(b)(2):*** ***(i)*** *Plot of eigenvalues in the order of decreasing value, i.e., λ_k as a function of k.* ***(ii)*** *Same plot as in (i) with eigenvalues on a logarithmic scale, i.e., plot of $\ln(\lambda_k)$ versus k.* ***(iii)*** *Plot of ρ_k, the fraction of variance explained, as a function of k.*

(3) [5pts] The plot of ρ_k, the fraction of variance explained by the top k principal components, as a function of k is shown in Figure 2(iii). As expected, as k increases, ρ_k increases. It reaches the 90% mark close to $k = 100$.

(4) [5pts] The smallest values of k for which $\rho_k \geq 0.51, 0.75, 0.90, 0.95$, and 0.99 are $k = 6, 29, 105, 179$, and 300, respectively.

(c) [9pts] ☕ *(Image Approximation through PCA)* The first eigenface corresponds to the largest eigenvalue and represents a direction that encompasses the largest variance in the training data, the second eigenface corresponds to the second largest eigenvalue and represents a direction which is orthogonal to the first eigenface and encompasses the second largest variance in the training data, and so on. A linear combination of eigenfaces along with a mean face, can be used to reconstruct a given face. Specifically, let $\mathbf{x}$ denote the vectorized representation of an image. An approximation to $\mathbf{x}$ based on the top k principal components is given by

$$\hat{\mathbf{x}} = \hat{\boldsymbol{\mu}}_x + \sum_{i=1}^{k} \hat{y}_{i,PCA} \cdot \mathbf{u}_i, \quad \text{where} \quad \hat{y}_{i,PCA} = \mathbf{u}_i^\top(\mathbf{x} - \hat{\boldsymbol{\mu}}_x)$$

[1pt per image] Generate a single figure (using subplots) showing the following: the mean face, the k principal component approximation face for image #43 in the face dataset for $k = 1$, $k = 2$, all the k values that you found in part (b) sub-part (4), and then show the original image in the same figure too. Add a descriptive title to each image in the figure and a title to the overall figure.

Solution: Image #43 and its k principal component approximation for different values of k are shown in Figure 3.

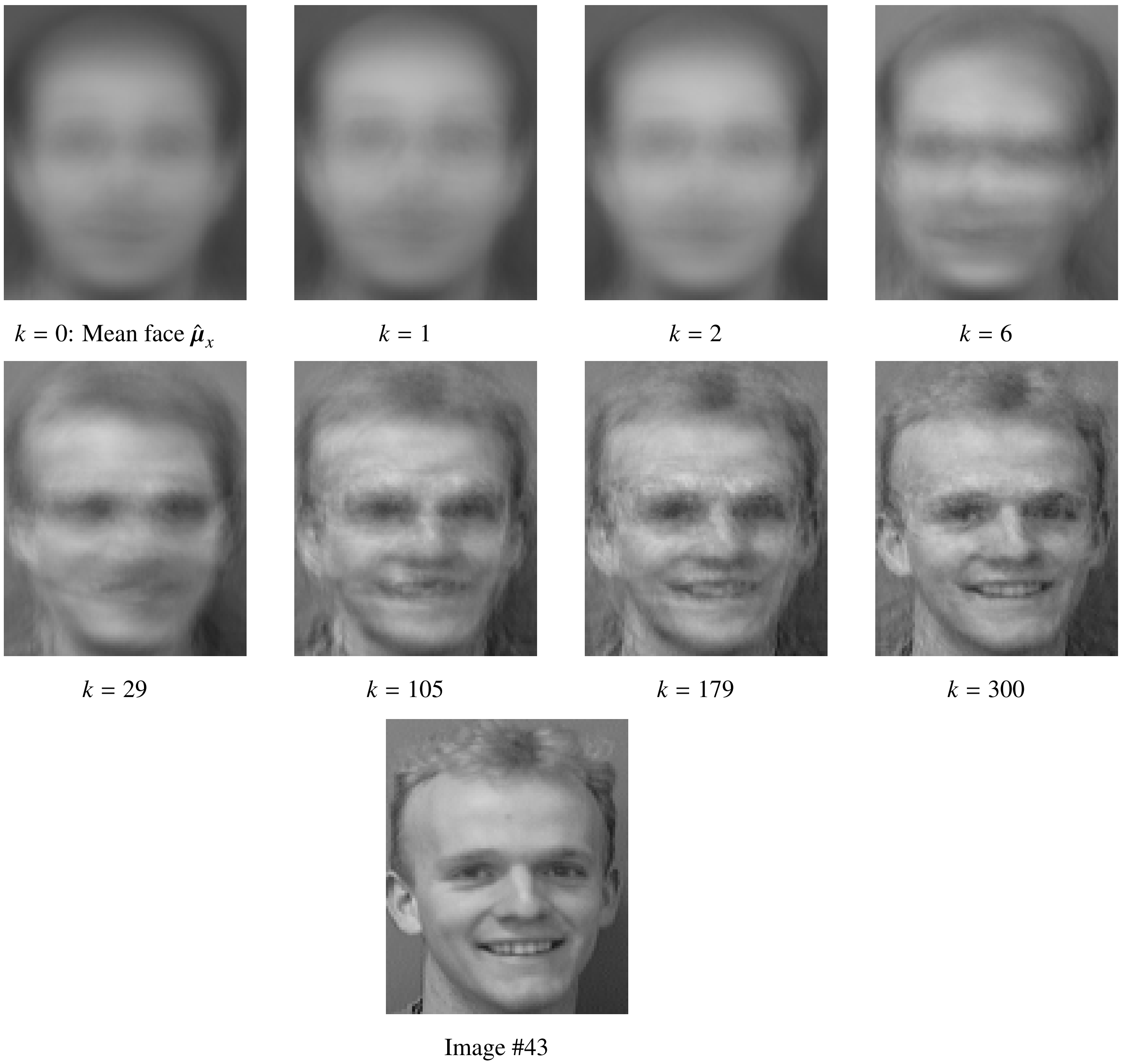


Figure 3: ***Problem 9.2(c):*** *Image #43 and its k principal component approximation for different k values.*