1. Conceptual questions [20 + 5 points].

1. (5 points) Please prove the first principle component direction v corresponds to the largest eigenvector of the sample covariance matrix:

$$v = \arg\max_{w:||w||<=1} \frac{1}{m} \sum_{i=1}^{m} (w^T x^i - w^T \mu)^2$$

You may use the proof steps in the lecture, but please write them logically and cohesively.

Answer: The formual above states we are looing for the direction of w (or weight vector) such that the variance of the data along direction w is maximized & less than or equal to 1. Here $w^T x^i$ is the projected data, reative to the mean: $w^T \mu$

First, we use linear algebra to manipulate the objective:

$$\frac{1}{m} \sum_{i=1}^{m} (w^T x^i - w^T \mu)^2$$

$$= \frac{1}{m} \sum_{i=1}^{m} (w^T (x^i - \mu))^2$$

$$= \frac{1}{m} \sum_{i=1}^{m} (w^T (x^i - \mu) w^T (x^i - \mu))$$

$$= \frac{1}{m} \sum_{i=1}^{m} w^T (x^i - \mu)(x^i - \mu)^T w$$

$$= w^T \underbrace{\left(\frac{1}{m} \sum_{i=1}^{m} (x^i - \mu)(x^i - \mu)^T \right) w}_{C}$$

We see the covariance matrix, C, is part of the equation, above, as noted. Therefore we can rewrite this equation as:

$$\max\ w^T C w$$
$$||w|| <= 1$$

The direction is represented by w, which should maximize variance. To solve the PCA problem, it becomes a constrained optimization problem. The general approach for solving optimization problems is using the Lagrangian function, which we apply to the equation from above:

$$L(w, \lambda) = w^T Cw + \lambda(1 - ||w||^2)$$

We use the Lagrangian multiplier λ to create some violation. What is the corresponding w that we will achieve by solving this optimization problem? We maximize the Lagrangian function with respect to w, while minimizing it with respect to λ.

If w is a maximum of the original optimization problem, then there exists a λ, where (w, λ) is a stationary point of $L(w, \lambda)$.

How to do this: Use multivariate calculus to get the derivatives of parts of the previous equation:

$$\delta w^T Cw = 2Cw$$
$$\delta||w||^2 = 2w$$

Take the derivative of the Lagrangian function, set it equal to zero. This implies that:

$$\frac{\delta L}{\delta w} = 0 = 2Cw - 2\lambda w <=> Cw = \lambda w$$

We see we end up with an eigendecomposition probem, with w the eigenvector and λ the eigenvalue for C.

Objective function becomes λ or eigen-value (associated with w)

$$w^T Cw = \lambda w^T w = \lambda||w||^2$$

Furthermore, it is apparent that the largest eigenvector is the weight vector required for the first principle component direction, as Cw = λw. The reason for this is that the λ value which maximizes the objective function, or variance, is the largest eigenvalue.

The problem becomes finding the largest eigenvalue of C.

The optimal solution w should be an eigen-vector of C. By choosing w_1 or the largest eigen-vector of C, the coresponing largest eigen-value, or variance, is λ_1.

Thus, we compute the reduced representations or principle components, of a data point as follows:

$$z^i = w^{i^T}(x^i - \mu)/\sqrt{\lambda_i}$$

The first principle component direction v corresponds to the largest eigenvector of the the sample covariance matrix, written as z^i:

$$z^1 = w^{1^T}(x^1 - \mu)/\sqrt{\lambda_1}$$

Source: pca.pdf, Xie, Yao, Ph.D., Associate Professor, Georgia Institute of Technology

2. (5 points) Based on your answer to the question above, explain how to further find the second largest principle component directions.

To get the second largest principle component direction, we simply take the next largest eigen-vector & eigen-value pair of C, or w_2 eigen-vector or direction, & coresponing next largest eigen-value or variance of λ_2, with the constraints that the second principle component is orthogonal to the first.

Building on the equation above, the equation for the second largest principle component is:

$$z^2 = w^{2^T}(x^2 - \mu)/\sqrt{\lambda_2}$$

We recall that in solving an eigenvalue problem, such as this one, there will be multiple solution: $w_1, w_2, w_3, \ldots$, the eigenvectors or directions of C, with correspondin eigenvalues or variance of $\lambda_1, \lambda_2, \lambda_3 \ldots$ The eigenvectors are ortho-normal.

3. (5 points) Based on the outline given in the lecture, show that the maximum likelihood estimate (MLE) for Gaussian mean and variance parameters are given by

$$\hat{\mu} = \frac{1}{m}\sum_{i=1}^{m} x^i, \hat{\sigma}^2 = \frac{1}{m}\sum_{i=1}^{m}(x^i - \hat{\mu})^2$$

,

respectively. Please show the work for your derivations in full detail.

Let us begin by an overview of the approach to reaching the estimation of parametric models.

We begin by assuming m data points $D = \{x^1, x^2, \ldots x^m\}$, iid & from an unnown distribution $P^*(x)$. We want to fit the data wiht the model $P(x|\theta)$, w/ parameters θ

$$\theta = argmax_\theta log P(D|\theta)$$

θ is the maximizer to solve this optimization problem. Alter θ to increase the probability of seeing the data.

Take the log, which is written as the product of the distribution.

$$\hat{\theta} = argmax_\theta log \prod_{i=1}^{m} P(x^i|\theta)$$

After introducing the log the product becomes the sum, which simplifies finding the gradient. (Using the sum instead of the product simplifies the problem)

$$\hat{\theta} = argmax_\theta \sum_{i=1}^{m} log P(x^i|\theta)$$

In a similar fashion, we begin the step by step process to show that the maximum likelihood estimate (MLE) for Gaussian mean and variance parameters are given by the equation presented in question 3, above.

We start with the equation for the Gaussian distribution in R

$$p(x|\mu,\sigma) = \frac{1}{(2\pi)^{\frac{1}{2}}\sigma} exp\left(-\frac{1}{2\sigma^2}(x-\mu)^2 \right)$$

We apply the log, which gives the following:

$$\mu, \sigma = argmax \sum_{i=1}^{N} logp(x_i|\mu,\sigma) = argmax \sum_{i=1}^{N} log \frac{1}{\sqrt{2\pi\sigma}} exp\left(-\frac{(x_1-\mu)^2}{2\sigma^2} \right)$$

Simplify the expression inside the log, (property 1)

$$\mu, \sigma = argmax \sum_{i=1}^{N} log(1) - log(\sqrt{2\pi}) - log(\sigma) - \frac{(x_1-\mu)^2}{2\sigma^2}$$

Remove constants not influenced parameters μ, σ :

$$\mu, \sigma = argmax \sum_{i=1}^{N} -log(\sigma) - \frac{(x_1-\mu)^2}{2\sigma^2}$$

Change the sign & turn the maximization problem into a minimization problem (standard notation):

$$\mu, \sigma = argmin \sum_{i=1}^{N} log(\sigma) + \frac{(x_1-\mu)^2}{2\sigma^2}$$

Substitute the objective function:

$$J(\mu, \sigma) = \sum_{i=1}^{N} log(\sigma) + \frac{(x_1-\mu)^2}{2\sigma^2}$$

Or:

$$\mu, \sigma = argmin \sum_{i=1}^{N} J(\mu, \sigma)$$

Find the parameters μ, σ: calculate the partial derivatives and set to zero:

$$\frac{\partial}{\partial \mu} J(\mu, \sigma) = 0- > \mu$$

$$\frac{\partial}{\partial \sigma} J(\mu, \sigma) = 0- > \sigma$$

A. Partial derivative for μ:

$$\frac{\partial}{\partial \mu} J(\mu, \sigma) = 0$$

$$\frac{\partial}{\partial \mu} \sum_{i=1}^{N} log(\sigma) + \frac{(x_1 - \mu)^2}{2\sigma^2} = 0$$

$$\sum_{i=1}^{N} \frac{2(x_1 - \mu)(-1)}{2\sigma^2} = 0$$

$$2\left(\sum_{i=1}^{N} x_i - \sum_{i=1}^{N} \mu \right) = 0$$

$$\sum_{i=1}^{N} x_i = \sum_{i=1}^{N} \mu$$

$$\sum_{i=1}^{N} x_i = N\mu$$

$$\frac{1}{N} \sum^{N} x_i = \mu$$

B. Partial derivative for σ (variance):

$$\frac{\partial}{\partial \sigma} J(\mu, \sigma) = 0- > \sigma$$

$$\frac{\partial}{\partial \sigma}(-\frac{n}{2} log(2\pi\sigma^2) - \frac{1}{2\sigma^2} \sum_{i}^{n}(x_i - \mu)^2)$$

Set = to 0:

$$-\frac{n}{\sigma} + \frac{1}{\sigma^3} \sum_{i}^{n}(x_i - \mu)^2 = 0$$

Subtract the first term from each side & multiply by σ^3:

$$\sum_{i}^{n}(x_i - \mu)^2 = n\sigma^2$$

Divide each sideby n:

$$\frac{1}{N}\sum_{i=1}^{N}(x^i - \mu)^2 = \hat{\sigma}^2$$

Put the partial derivatives for σ^2 & μ, found above, next to each other, add hats, so we have: $\hat{\sigma}^2$ & $\hat{\mu}$, switch equations from one side of the equal sign to the other, replace N with m, and we have proved that the maximum likelihood estimate (MLE) for Gaussian mean and variance parameters are given by

$$\hat{\mu} = \frac{1}{m}\sum_{i=1}^{m} x^i, \hat{\sigma}^2 = \frac{1}{m}\sum_{i=1}^{m}(x^i - \hat{\mu})^2$$

,

which is what question 1.3 asked us to prove.

Source: Lecture 6: Density estimation: Estimation of parametric models. Xie. Yao. Ph.D.. Associate

4. (5 points) Explain the three key ideas in ISOMAP (for manifold learning and non-linear dimensionality reduction).

ISOMAP key ideas:

– keep “walking distance” over the data cloud (manifold) by creating low dimensional representation.

– let A be the adjacency matrix recording neighbor Euclidean distance, & find neighbors $N(i)$ of each data point, x^i, within distance E.

– Based on A, determine the shortest path distance matrix D between pairs of points, $x^i and x^j$.

– Preserves distances information in D by finding low dimensional representation.

Source: Nonlinear Dimensionality Reduction lecture, Xie, Yao, Ph.D., Associate Professor, Georgia Institute of Technology

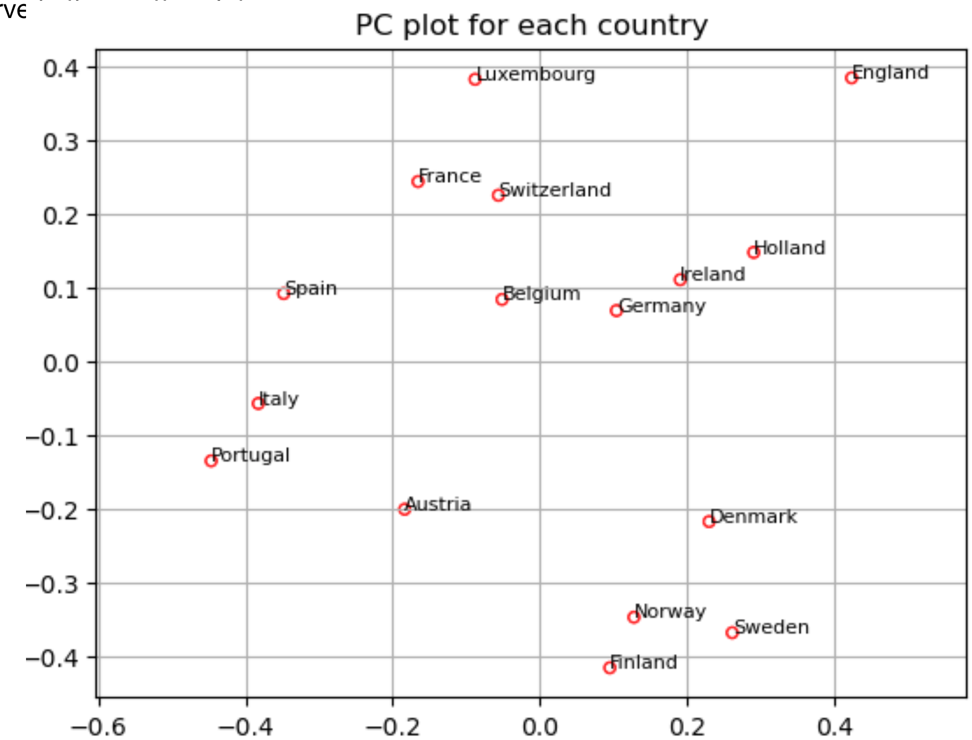
2.PCA: Food consumption in European countries [20 points].

The data “food-consumption.csv” contains 16 countries in Europe and their consumption for 20 food items, such as tea, jam, coffee, yogurt, and others. We will perform principal component analysis to explore the data.

(a) (10 points) For this problem of performing PCA on countries by treating each country’s food consumption as their “feature” vectors, explain how the data matrix is set-up in this case (e.g., the columns and the rows of the matrix correspond to what). Now extract the first two principal components for each data point (thus, this means we will represent each data point using a two-dimensional vector). Draw a scatter plot of two-dimensional representations of the countries using their two principal components. Mark the countries on the plot (you can do this by hand if you want). Please explain any pattern you observe

The data matrix is set-up in this case such that the matrix is of the form mxn, with the 16 countries as m or rows, and the 20 foods as n, or columns. Relative food consumption styles of each country are illustrated in the scatter plot chart, right.

Interestingly, food preferences by country appear to follow patterns somewhat related to a country's geographical proximity to another country, although there are some exceptions.



The map, above, helps to illustrate this theory.

Examples of countries with similar food preferences to their geographic neighbors are the countries Denmark, Sweden, Norway and Finland; Holland, Germany and Belgium; Switzerland and France, with Luxembourg not far away. England’s distance from other countries on this chart follows the geographic proximity logic, as it is an island, physically separated by water from the continent.

As mentioned, there are exceptions that do not follow the theory that countries’ food preferences proximity on this chart corresponds to geographic proximity. For example, on the chart, Ireland is close to Holland and Germany; Italy and Portugal are close, with Spain more distant from Portugal. Austria is as isolated as England on the chart, despite the fact that a large part of its borders are shared with other countries in this analysis.

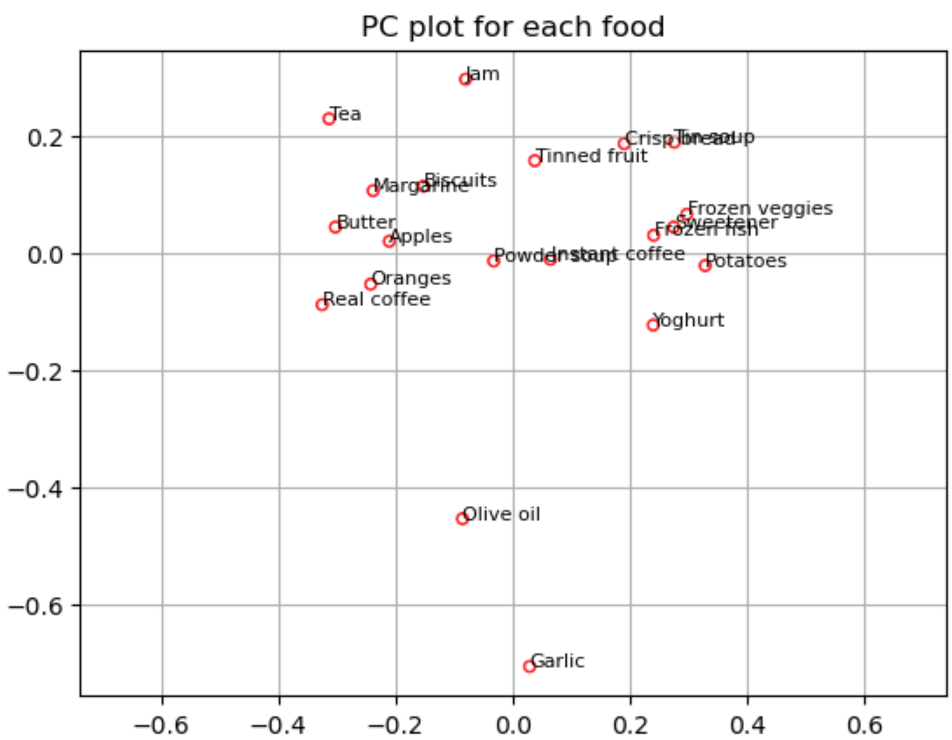
It is possible a study of ancient European history regarding who settled different areas at various times, as we as old maps showing countries that were once one, might offer insight into some of these discrepancies. For example, Austria, while it does not have similar food preferences with countries it borders to the West, might share food preferences with those to its East. Climate, proximity to the ocean and economic factors might impact these groupings as well.

2.PCA: Food consumption in European countries [20 points]. (cont.)

b) **(10 points) Now, we will perform PCA analysis on the data by treating country consumptions as “feature” vectors for each food item**. In other words, we will now find weight vectors to combine country consumptions for each food item to perform PCA another way. Project data to obtain their two principle components (thus, again each data point – for each food item – can be represented using a two-dimensional vector). Draw a scatter plot of food items. Mark the food items on the plot (you can do this by hand if you want). Please explain any pattern you observe in the scatter plot.

The groupings of food in the “Food Principal Component Plot” is somewhat similar to groupings of Market Basket analysis. In both cases, items are grouped with other items a person would eat together, for the most part. Fc example, it’s logical to buy butter, margarine an biscuits together; apples and oranges together; crisp bread and soup; instant coffee and powdered soup; frozen vegetables and frozen fish.

In some cases, the frequency with which some items are bought, may relate to the food’s shelf life. For example: olive oil. I would think this would be used for cooking throughout all countries in this analysis. Yet because it is only needed in small amounts, comes in a large bott and has a long shelf life, it does not need to be bought as frequently as many of the other items such as apples and oranges. Items bought less frequently should have a negative X and Y valu in this analysis.

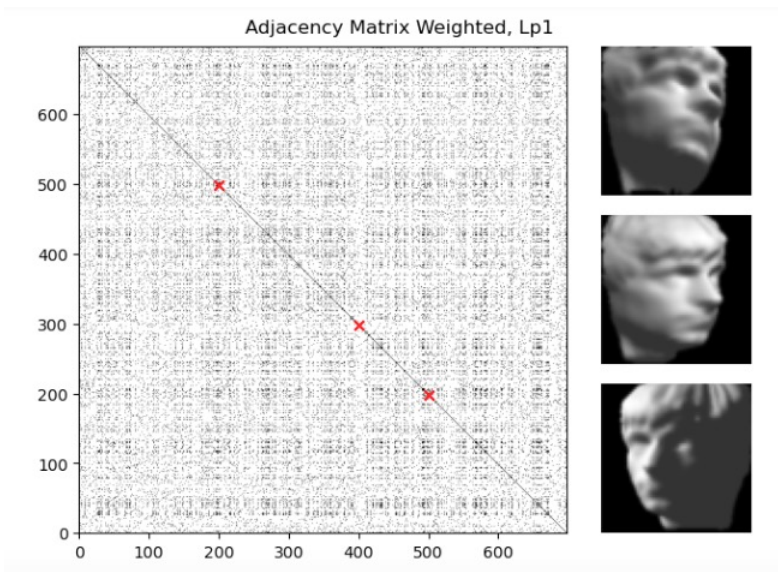


3. Order of faces using ISOMAP [25 points]

This question aims to reproduce the ISOMAP algorithm results in the original paper for ISOMAP, J.B. Tenenbaum, V. de Silva, and J.C. Langford, Science 290 (2000) 2319-2323 that we have also seen in the lecture as an exercise (isn’t this exciting to go through the process of generating results for a high-impact research paper!) The file isomap.mat (or isomap.dat) contains 698 images, corresponding to different poses of the same face. Each image is given as a 64 × 64 luminosity map, hence represented as a vector in R4096.

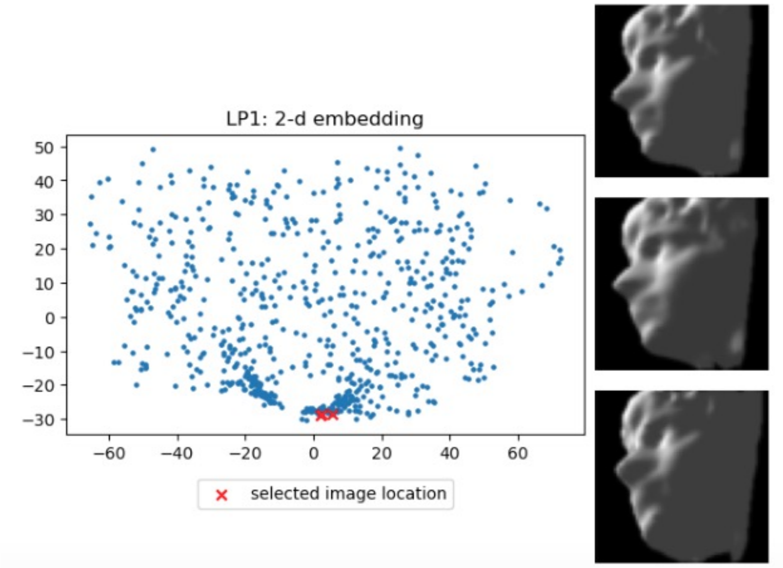
(a) (5 points) Visualize the nearest neighbor graph (you can either show the adjacency matrix (e.g., as an image), . . . and illustrate a few images corresponds to nodes at different parts of the graph, e.g., mark them by hand or use software packages.

Weighted adjacency matrix, right. The distance to the nearest neighbor graph is represented by each entry. The randomly selected images, pictured to the right, have their locations marked with the red crosses.



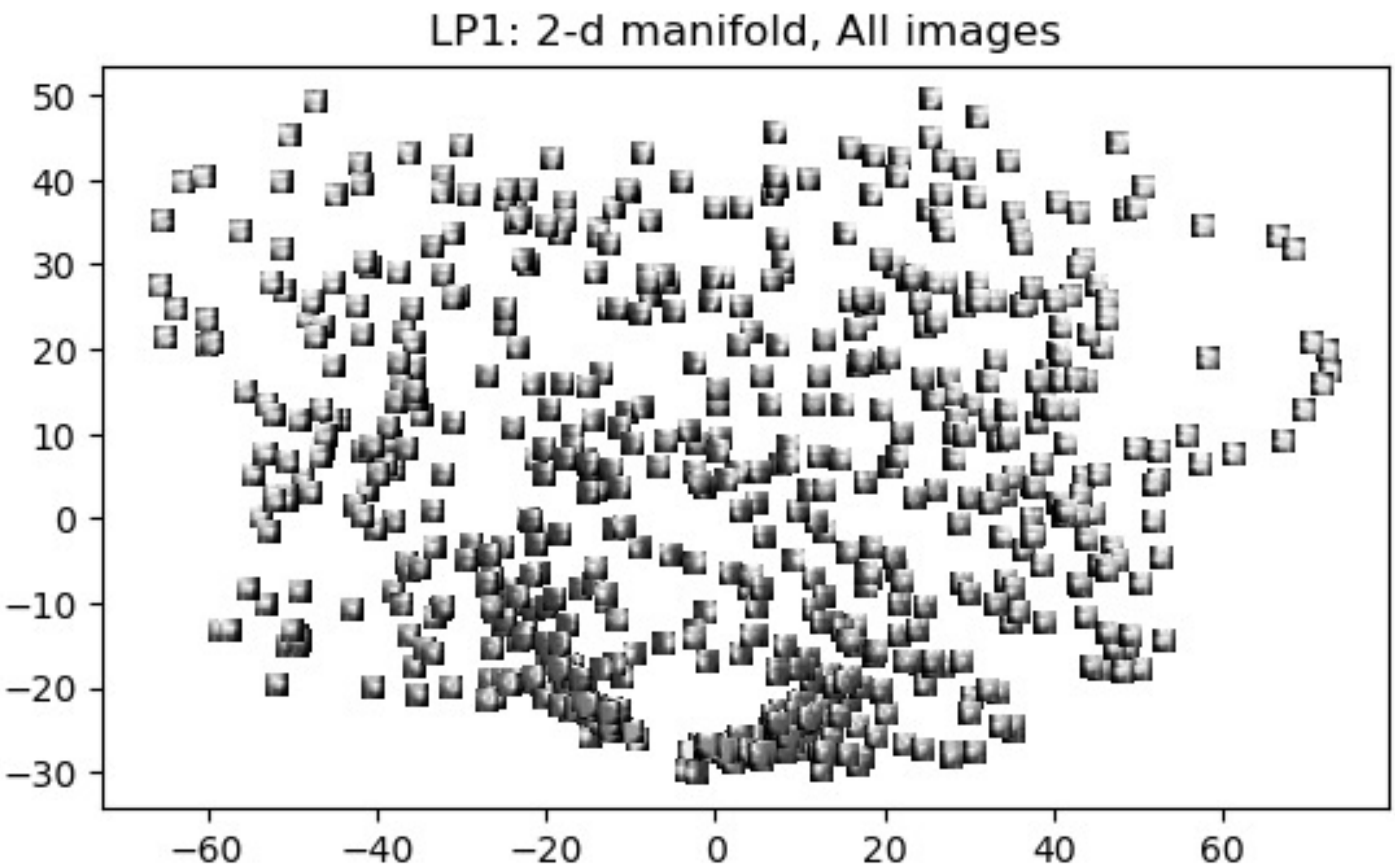
3. Order of faces using ISOMAP [25 points] (cont.)

(b) (15 points) Implement the ISOMAP algorithm yourself to obtain a two-dimensional low-dimensional embedding. Plot the embeddings using a scatter plot, similar to the plots in lecture slides. Find a few images in the embedding space and show what these images look like and specify the face locations on the scatter plot. Comment on whether or not you see any visual similarity among them and their arrangement, similar to what you saw in the paper?



2-D embedding plots, right. The randomly selected images, pictured to the right, have their locations marked with the red crosses.

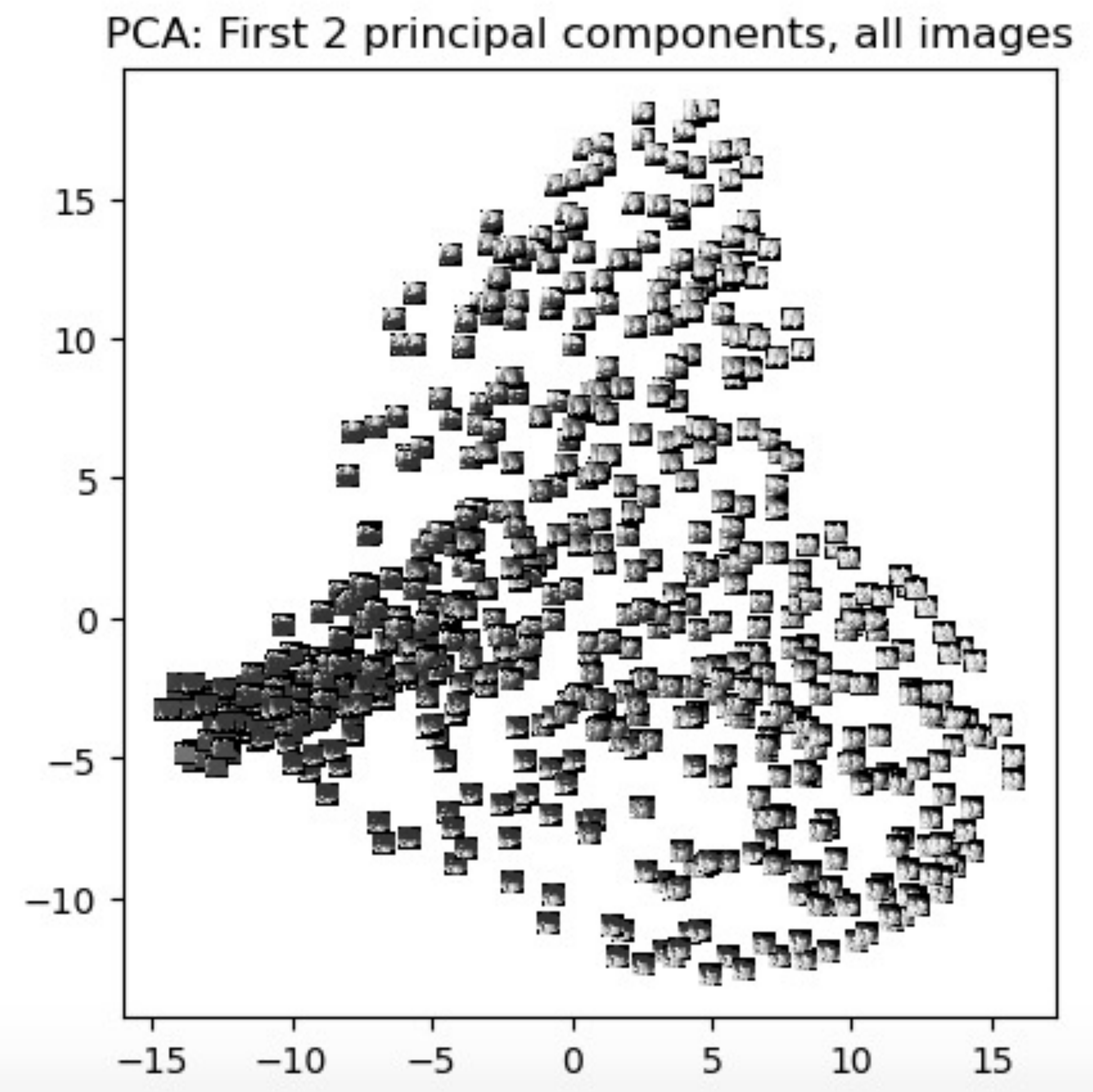
Yes, there are similarities among the images and their arrangements, to observations noted in the paper. For example, we notice a gradual change in direction that the poses are facing as we move along the manifold. There is a 'drifting' change in these faces globally, both here and as was noted in the paper.



3.Order of faces using ISOMAP [25 points] (cont.)

(c) (10 points) Perform PCA (you can now use your implementation written in Question 1) on the images and project them into the top 2 principal components. Again show them on a scatter plot. Explain whether or you see a more meaningful projection using ISOMAP than PCA.

We see a more meaningful projection with ISOMAP compared to PCA. Locally, the PCA embedded faces do show similarity. However PCA does not capture a 'drifting' change globally of the faces in the manifold.



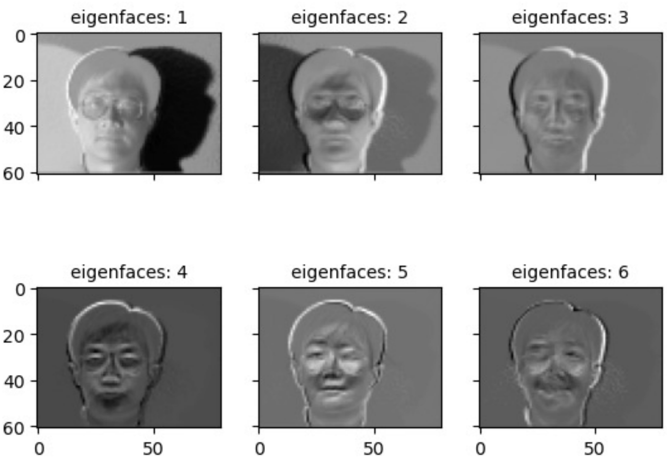
4. Eigenfaces and simple face recognition [25 points].

This question is a simplified illustration of using PCA for face recognition. We will use a subset of data from the famous Yale Face dataset.

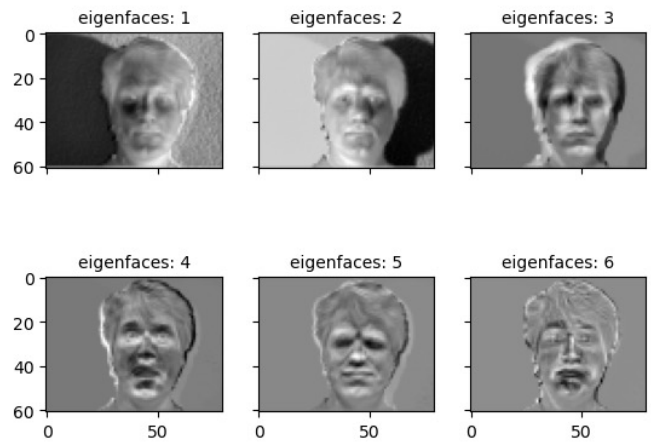
(a)(10 points) Perform analysis on the Yale face dataset for Subject 1 and Subject 2, respectively, using all the images EXCEPT for the two pictures named subject01-test.gif and subject02-test.gif. Plot the first 6 eigenfaces for each subject. When visualizing, please reshape the eigenvectors into proper images. Please explain can you see any patterns in the top 6 eigenfaces?

Following are the first six eigenfaces for subject 1 and 2. We noticed images associated with higher eigenvalues show a greater clarity of the features, and thus allow for greater recognition.

Eigenfaces for subject 1



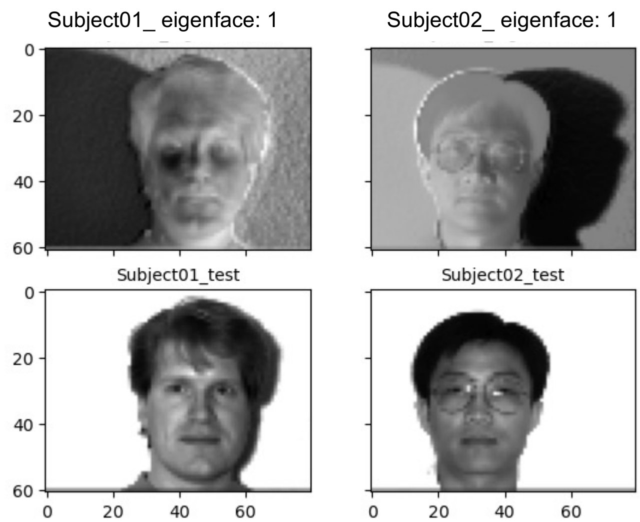
Eigenfaces for subject 2



(b) (10 points) Face recognition task.
Face recognition through PCA is proceeded as follows. Given the test image subject01-test.gif and subject02-test.gif, first downsize by a factor of 4 (as before), and vectorize each image. Take the top eigenfaces of Subject 1 and Subject 2, respectively. Then we calculate the projection residual of the 2 vectorized test images with the vectorized eigenfaces:

$$s_{ij} = \|(\text{test image})_j - (\text{eigenface}_i)(\text{eigenface})^T_i(\text{testmage})_j\|_2^2$$

Report all four scores: s_{ij} , $i = 1, 2$, $j = 1, 2$. Explain how to recognize the faces of the test images using these scores.



Recognition should be calculated by choosing the eigenface with a lower residual / errors with the test image. For this analysis that was true for subject 1, but not subject 2.

	test 1	test 2
eg_face_1	9.700357e+11	1.048548e+12
eg_face_2	9.703570e+11	1.048716e+12

(c) (5 points) Comment if your face recognition algorithm works well and discuss how you would like to improve it if possible.

As noted above, this face recognition algorithm did not work well, as it was correct only 50% of the time. To improve this, I would like to try the normalized inner product score.

5. To subtract or not to subtract, that is the question [10 points].

We proved in 1.1, above, that the first principle component direction v corresponds to the largest eigenvector of the the sample covariance matrix, w^1, written as z^i:

(a)

$$z^i = w^{1^T}(x^i - \mu)/\sqrt{\lambda_1}$$

Or:

$$z^1 = w^{1^T}(x^1 - \mu)/\sqrt{\lambda_1}$$

$$z^1 = w^T(x^1 - \mu)/\sqrt{\lambda_1} = 5$$

Now suppose Prof. X insists not subtracting the mean. Following the steps illustrated in the answer to 1.1, above, the result to finding the largest eigenvector of the the sample covariance matrix, w^1, written as z^i: would be similar to (a), but without subtracting the mean. This would result in:

(b)

$$z^i = w^{1^T} x^i/\sqrt{\lambda_1}$$

$$z^1 = w^T x^1/\sqrt{\lambda_1}$$

Clearly, these two equations are not equal

$$w^T x^1/\sqrt{\lambda_1}! = w^T(x^1 - \mu)/\sqrt{\lambda_1}$$

Answer: No, with and without subtracting the mean are not will result in equal eigenvectors.