CIS 520, Machine Learning, Fall 2021
Homework 6
Due: Tuesday, October 26th, 11:59pm
Submit to Gradescope

Instructions. Please write up your responses to the following problems clearly and concisely. We require you to write up your responses using LaTeX; we have provided a LaTeX template, available on Canvas, to make this easier. **Submit your answers in PDF form to Gradescope. We will not accept paper copies of the homework.**

Collaboration. You are allowed and encouraged to work together. You may discuss the **written homework** to understand the problem and reach a solution in groups. However, **it is recommended that each student also write down the solution independently and without referring to written notes from the joint session.** You must understand the solution well enough to reconstruct it by yourself. (This is for your own benefit: you have to take the exams alone.)

Learning Objectives

After completing this assignment, you will be able to:

- Understand the relationship between singular values/vectors and eigenvectors/values
- Understand the relationship between PCA reconstruction error and eigenvalues

Deliverables

This homework can be completed individually or in groups of 2. You need to make one submission per group. Make sure to add your team member's name on Gradescope when submitting the homework's written and coding part.

1. **A PDF compilation of `hw6.tex` with team member's names in the agreement**
2. **A link to `hw6.ipynb` on Colab with required code implemented**

1 Singular Value Decomposition [40 points]

1. **[15 points]** Let $\mathbf{X}$ be an n by p matrix. Show that if $\mathbf{X}$ has rank p (all its columns are linearly independent) and $n > p$, then $\widehat{\mathbf{w}} = \mathbf{X}^{+}\mathbf{y}$ using the p-dimensional pseudo-inverse $\mathbf{X}^{+} = \mathbf{V}_k \Lambda_k^{-1} \mathbf{U}_k^T$ with $k = p$ solves the least squares problem $\widehat{\mathbf{w}} = \arg\min_w (\mathbf{y} - \mathbf{X}\mathbf{w})^T (\mathbf{y} - \mathbf{X}\mathbf{w})$.

   Hint: A useful matrix derivative identity is: $\frac{\partial}{\partial \mathbf{s}}(\mathbf{x} - \mathbf{A}\mathbf{s})^T(\mathbf{x} - \mathbf{A}\mathbf{s}) = -2\mathbf{A}^T(\mathbf{x} - \mathbf{A}\mathbf{s})$.

2. **[20 points]** Let $\mathbf{X}$ be an n by p matrix. Given the unit eigenvectors of $\mathbf{X}\mathbf{X}^T$ as $(\mathbf{u}_1, ..., \mathbf{u}_n)$ and corresponding eigenvalues as $(\lambda_1, ..., \lambda_n)$, give an expression for computing a unit eigenvector $\mathbf{v}_i$ of $\mathbf{X}^T\mathbf{X}$ in terms of $\mathbf{X}$, $\mathbf{u}_i$, and λ_i.

   Hint: First prove that $\mathbf{X}\mathbf{X}^T$ *and* $\mathbf{X}^T\mathbf{X}$ *have the same non-zero eigenvalues.*

3. **[5 points]** Let $\mathbf{X}$ be an n by p matrix. Under what condition (in terms of the relationship between n and p) would the result from part 1.2 be an efficient way to find the largest eigenvectors of $\mathbf{X}^T\mathbf{X}$? Explain your reasoning.

2 Simple Principal Component Analysis [30 points]

In this assignment, we will implement Principal Component Analysis and perform it on a simple 2-dimensional dataset. First fill out the helper functions provided to retrieve covariance matrices, eigenvectors/values, and component projections. Use these helper functions to implement a PCA function.

2.1 Part 1: Comparing Principal Components

1. **[6 points]** Report the eigenvectors and eigenvalues here.

2. **[4 points]** What can you say about the relationship between the first principal component and the second?

2.2 Part 2: Plotting Principal Components in Original Space

1. **[6 points]** Plot the given points (with both axes in the same scale) as well as the arrows representing the principal components in original space, with x1 in the x-axis and x2 in the y-axis. The principal component arrows should originate at the mean and have magnitudes equal to their corresponding eigenvalues.

2. **[4 points]** Describe how the principal components relate to the points in terms of variance.

2.3 Part 3: Plotting Data Projected onto Component Space

1. **[6 points]** Now plot the given points (with both axes in the same scale) in principal component space, with x-axis representing the projection of the first component and the y-axis representing the component on the second.

2. **[4 points]** Explain how the graph of points on principal component space relates to the graph of points on original space above.

3 Principal Component Analysis on Faces [30 points]

Now we will perform PCA on images of faces and see how reducing the latent dimensions of our images affects the images reconstructions. First, start by uncommenting the code below to retrieve the faces dataset.

3.1 Part 1: PCA with SVD and Eigenfaces

1. [**3 points**] Report the first five singular values here.
2. [**3 points**] Paste the eigenfaces output here.
3. [**4 points**] Describe what the eigenfaces look like. What do you expect to observe with the eigenfaces associated with larger eigenvalues?

3.2 Part 2: Reconstructing Faces

1. [**4 points**] Paste the portrait reconstructions here.
2. [**3 points**] Compare the reconstructed images to the original images. How are they similar and how are they different? Shortly explain why they are different.
3. [**3 points**] What do you expect to see from the reconstructed images as the number of principal components chosen for PCA increases? Please explain why.

3.3 Part 3: Variance Explanation

1. [**4 points**] Insert the three plots of explanation vs. number of components, descending eigenvalues vs. number of components, and reconstruction error vs. number of components here.
2. [**3 points**] How do you expect (based on theory; please be precise!) the plot of variance explained as the number of components to relate to the eigenvalues of the corresponding components?
3. [**3 points**] What is the relation between reconstruction error and the variance explained?