The objective of this lab is for you to program PCA and LDA in Matlab and apply them to some datasets. The TA will first demonstrate the results that PCA and LDA give on the MNIST dataset. Then, you will program them, replicate those results, and further explore other datasets. You can use the textbook, lecture notes and your own notes, as well as the Matlab functions we provide in the course web page.

I Datasets

You will use the MNIST dataset of handwritten digits $O \downarrow 2 3 4 5 6 7 8 9$. PCA will need the instances $\mathbf{x} \in \mathbb{R}^D$ (where D = 784), while LDA will need both the instances and their labels $y_n \in \{0, \ldots, 9\}$. You will need to plot instances as grayscale images of 28×28 , as seen in previous labs; and "eigendigits" as color images of 28×28 . You will also need to plot reduced-dimension instances $\mathbf{z}_n \in \mathbb{R}^L$ (where L is 1D, 2D or 3D) as scatterplots; color them differently for each class (even if the class information was not used for training), so we can tell them apart.

Additionally, you will apply PCA and LDA to:

- The rotated-7 MNIST dataset **E CONTROL CONTROL**. Each digit '7' should be considered as a class containing all its rotated versions. Ignore the "skeleton" data in the file, just use the images and the class labels.
- One other dataset of your choice. For example, from the UCI repository, or a dataset of face images (several are available in the Internet).

II Implementing and using PCA

Important: when developing and testing your code, use toy examples for which you know the true solution ahead of time (e.g. generate points along a line in 3D and add noise to them, then reduce to 1D or 2D with PCA). Once your code works well there, try it on more difficult datasets. The following Matlab functions will be useful (among others): mean cov eig sort find linspace.

- Assume a matrix **X** of $D \times N$ (instances = columns).
- Start by computing the mean μ and covariance Σ of the data. Program this using loops, then check the result with the Matlab functions mean and cov.
- Program PCA by computing the eigendecomposition of the covariance matrix $\Sigma = U\Lambda U^T$ and setting $W = U_{1:L}$.
- Program how to project a point $\mathbf{x} \in \mathbb{R}^D$ onto the *L* principal component subspace (where $1 \leq L \leq D$), and how to reconstruct a vector $\mathbf{z} \in \mathbb{R}^L$ into the original, data space. This is given by the PCA projection mapping $\mathbf{z} = \mathbf{F}(\mathbf{x}) = \mathbf{W}^T(\mathbf{x} - \boldsymbol{\mu})$ and the reconstruction mapping $\mathbf{x}' = \mathbf{f}(\mathbf{z}) = \mathbf{W}\mathbf{z} + \boldsymbol{\mu}$, respectively.
- Verify that the covariance matrix in the projected space (that is, $\operatorname{cov} \{\mathbf{z}_1, \ldots, \mathbf{z}_N\}$) equals $\mathbf{W}^T \Sigma \mathbf{W}$, that it is diagonal, and that the sum of its diagonal elements equals $\lambda_1 + \cdots + \lambda_L$.
- Plot the following figures:
 - 1. The eigenvalues $\lambda_1, \ldots, \lambda_D$ and the proportion of explained variance $\frac{\lambda_1 + \cdots + \lambda_L}{\lambda_1 + \cdots + \lambda_D} \in [0, 1]$ as a function of the number of dimensions used L (as in the textbook fig. 6.4).
 - 2. The mean μ , as a grayscale image.
 - 3. The MNIST dataset projected onto 2D (as in the textbook fig. 6.5). Use different colors/markers for different digit classes, so we can recognize them.
 - 4. The MNIST dataset projected onto 3D, colored as in the 2D plot.
 - 5. The eigenvectors $\mathbf{u}_1, \ldots, \mathbf{u}_L \in \mathbb{R}^D$, as color images ("eigendigits").
 - 6. A vector **x** and its reconstruction $\mathbf{x}' = \mathbf{W}(\mathbf{W}^T(\mathbf{x} \boldsymbol{\mu})) + \boldsymbol{\mu}$, both as grayscale images.
 - 7. Vectors of the form $\boldsymbol{\mu} \pm \alpha \mathbf{u}_l$ for $\alpha > 0$ (where $1 \leq l \leq D$), as grayscale images. This shows what the *l*th principal component subspace corresponds to in data space. It is equivalent to reconstructing vectors $\mathbf{z} \in \mathbb{R}^L$ that move along the *l*th PC axis.

Then, explore PCA in different settings:

- Compute PCA on only the digits 1s, then visualize it and reconstruct digits (1s, 2s, etc.). The projection on the first two PCs shows a clear structure, what does it correspond to? Why does the mean μ look the way it does?
- Compute PCA on the entire MNIST dataset (all digits), then visualize it and reconstruct digits.
- See the end of file lab03_pca.m for further suggestions.

III Implementing and using LDA

As with PCA, write code to compute LDA and plot relevant results:

- Assume a matrix **X** of $D \times N$ (instances = columns) and a vector **y** of $1 \times N$ (class labels in $1, \ldots, K$).
- Program how to compute the within-class and between-class scatter matrices \mathbf{S}_W and \mathbf{S}_B . You will find it convenient to add a small number to the diagonal of \mathbf{S}_W (e.g. $10^{-10} \operatorname{tr}(\mathbf{S}_W)/D$) to make \mathbf{S}_W be full rank.
- Program LDA by computing the eigendecomposition of $\mathbf{S}_{W}^{-1}\mathbf{S}_{B} = \mathbf{U}\mathbf{\Lambda}\mathbf{U}^{T}$ and setting $\mathbf{W} = \mathbf{U}_{1:L}$.
- Program how to project a point $\mathbf{x} \in \mathbb{R}^D$ onto the LDA subspace of dimension L (where $1 \leq L \leq K 1$). This is given by the LDA projection mapping $\mathbf{z} = \mathbf{F}(\mathbf{x}) = \mathbf{W}^T \mathbf{x}$.
- Plot the following figures:
 - 1. The eigenvalues $\lambda_1, \ldots, \lambda_D$ and the proportion of explained variance $\frac{\lambda_1 + \cdots + \lambda_L}{\lambda_1 + \cdots + \lambda_D} \in [0, 1]$ as a function of the number of dimensions used L (as in the textbook fig. 6.4).
 - 2. The mean of each class μ_k , as a grayscale image.
 - 3. The MNIST dataset projected onto 2D (as in the textbook fig. 6.12). Use different colors/markers for different digit classes, so we can recognize them.
 - 4. The MNIST dataset projected onto 3D, colored as in the 2D plot.
 - 5. The eigenvectors $\mathbf{u}_1, \ldots, \mathbf{u}_L \in \mathbb{R}^D$, as color images ("Fisherdigits").

Questions to consider:

- Explore the algorithm in different settings (see the PCA section), and with different numbers of classes (for MNIST: different digits).
- How does the result of LDA differ from that of PCA? In particular, observe the 2D projections and the eigendigits and Fisherdigits.
- How many eigenvalues are nonzero in LDA (and how many in PCA)? Why? Remember that LDA applies if \mathbf{S}_W is invertible and $L \leq K - 1$.

IV What you have to submit

We have provided for you a script lab03_pca.m that loads the MNIST dataset, computes PCA and plots the figures mentioned earlier. So you only have to code LDA, not PCA. Then, you have to explore the behavior of both PCA and LDA with different datasets and different settings of the parameters.

Follow these instructions strictly. Email the TA the following packed into a single file (lab03.tar.gz or lab03.zip) and with email subject [CSE176] lab03:

• Matlab code for a script lab03_lda.m that implements LDA and produces relevant plots for the MNIST dataset. Use the provided lab03_pca.m as guide. The portion of the code that computes LDA should work with any dataset (not just MNIST) **X** of $D \times N$ with corresponding labels **y** of $1 \times N$ with K classes. You can make this its own function (e.g. lda(X,y,K)) or leave it inlined like the PCA computation in lab03_pca.m. Note: you are not allowed to use any functions from the Matlab Toolboxes (in particular, the Statistics and

Note: you are not allowed to use any functions from the Matlab Toolboxes (in particular, the Statistics and Machine Learning Toolbox, or the Neural Network Toolbox). You can only use basic Matlab functions.

• A brief report (2 pages) in PDF format describing your experience with 3 datasets: MNIST, rotated-7 MNIST and one other dataset of your choice. Make sure you understand the special structure of the rotated-7 MNIST dataset and how it differs from the regular MNIST.

The more extensive and insighful your exploration, the higher the grade. Be concise. Don't include code or figures, we can recreate them by running your functions. Indicate the part that each member of the group did.