Artificial Intelligence and Machine Learning

Exercises – Principal Component Analysis

Question 1 (Eigendecomposition of a symmetric matrix)

Let the square (and symmetric) matrix

$$\boldsymbol{A} := \begin{pmatrix} 3 & 1 & 1 \\ 1 & 2 & 2 \\ 1 & 2 & 2 \end{pmatrix} \in \mathbb{R}^{3\times 3}$$

be given. Please answer the following questions:

1. What are the eigenvalues of $\boldsymbol{A}$?
2. Compute the eigenspace for each eigenvalue. What do you observe?
3. Write down the eigendecomposition of $\boldsymbol{A}$, i. e. find the matrices $\boldsymbol{U} \in \mathbb{R}^{3\times 3}$ and $\boldsymbol{\Lambda} \in \mathbb{R}^{3\times 3}$ such that $\boldsymbol{A} = \boldsymbol{U}\boldsymbol{\Lambda}\boldsymbol{U}^\top$.

Question 2 ⊛

Which statements concerning PCA are **false**?

- ☐ The algorithm belongs to the category of supervised learning.
- ☐ The goal of PCA is to reduce the variance in the data as much as possible.
- ☐ The data is transformed linearly.
- ☐ All principal components are orthogonal.

Question 3 (Covariance matrix) ⊛

Let $\boldsymbol{\Sigma}$ be a covariance matrix. Which statements are correct?

- ☐ $\boldsymbol{\Sigma}$ is symmetric (i. e. $\boldsymbol{\Sigma}^\top = \boldsymbol{\Sigma}$).
- ☐ $\boldsymbol{\Sigma} \in \mathbb{R}^{M\times N}, M \neq N$.
- ☐ $\boldsymbol{\Sigma}$ is a square matrix.
- ☐ All entries on the main diagonal of $\boldsymbol{\Sigma}$ are non-negative.

Question 4 (Number of principal components) ⊛

Explain in up to three sentences how you can choose the number of principal components for dimensionality reduction. Name at least two different strategies!

Question 5 (PCA by hand) ⊛

You are presented with a 4-dimensional dataset. Your task is to reduce the dimensionality of the dataset as much as possible, while preserving at least 80 % of the original variance.

You have already computed the covariance matrix $\mathbf{\Sigma}$ and its eigendecomposition $\mathbf{\Sigma} = \boldsymbol{U}\mathbf{\Lambda}\boldsymbol{U}^\top$ in a previous step. You have found:

$$\underbrace{\begin{pmatrix} 4 & -2 & 3 & -1 \\ -2 & 4 & -3 & 1 \\ 3 & -3 & 5 & 0 \\ -1 & 1 & 0 & 5 \end{pmatrix}}_{\mathbf{\Sigma}} \approx \underbrace{\begin{pmatrix} -0.5 & 0.7 & -0.5 & 0 \\ 0.5 & 0.7 & 0.5 & 0 \\ -0.6 & 0 & 0.7 & -0.3 \\ 0.2 & 0 & -0.2 & -1 \end{pmatrix}}_{\boldsymbol{U}} \underbrace{\begin{pmatrix} 10 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 5 \end{pmatrix}}_{\mathbf{\Lambda}} \underbrace{\begin{pmatrix} -0.5 & 0.5 & -0.6 & 0.2 \\ 0.7 & 0.7 & 0 & 0 \\ -0.5 & 0.5 & 0.7 & -0.2 \\ 0 & 0 & -0.3 & -1 \end{pmatrix}}_{\boldsymbol{U}^\top}$$

Let D be the dimensionality of the reduced dataset. Determine D such that the constraint above is satisfied. Which vectors represent the principal components? *Please justify your answer.*

Question 6 (Eigenfaces)

Sklearn provides the *Labeled Faces in the Wild (LFW)* people dataset which comprises images of well known people's faces. Each image has a resolution of 50×37 pixels. The data can be loaded using the following commands:

```python
from sklearn.datasets import fetch_lfw_people

# GET DATA
# ------------------------------------------------------
lfw_people = fetch_lfw_people(
    min_faces_per_person=70, resize=0.4)

# get number of samples, height, and width of images
n_samples, h, w = lfw_people.images.shape

# get features
X = lfw_people.data
```

Remark: Each image is labeled with the name of the person shown. The labels can be loaded with the command `y = lfw_people.images.target`. However, we are not going to use these in this exercise. Figure 1 shows some sample images.

Work through the following tasks:

- Compute the mean face and the eigenfaces by performing an eigendecomposition of the covariance matrix of the data. For this you may want to use the function `np.linalg.eig()`.

- Plot the first thirty eigenfaces.

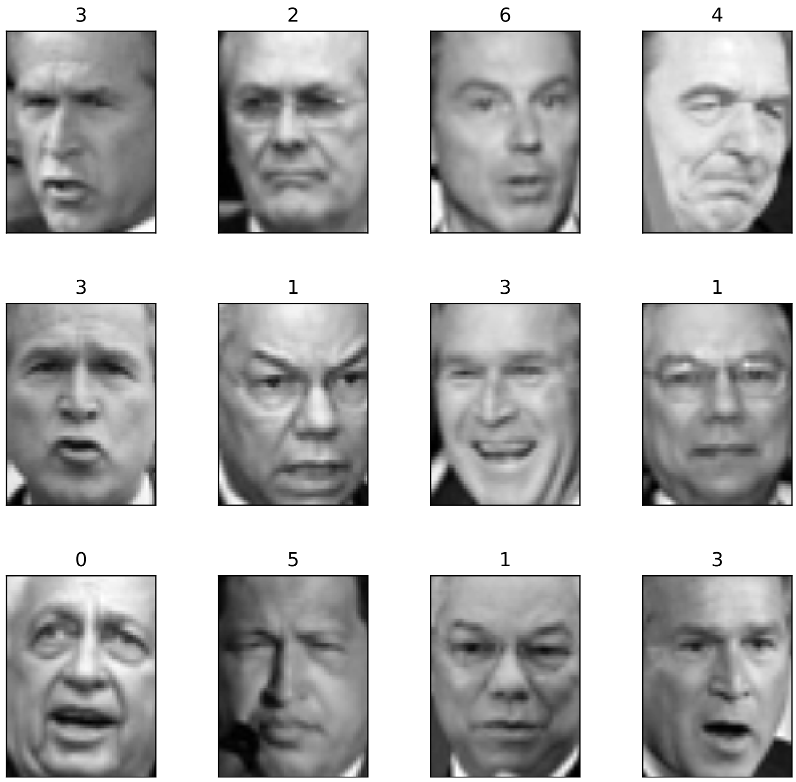

Figure 1: Some sample images from the LFW dataset.

Question 7 (FLDA)

Compute the derivative of the Fisher criterion

$$\mathfrak{J}_F(\boldsymbol{w}) = \frac{\boldsymbol{w}^\top \boldsymbol{S}_B \boldsymbol{w}}{\boldsymbol{w}^\top \boldsymbol{S}_W \boldsymbol{w}}$$

with respect to $\boldsymbol{w}$ and derive the generalized eigenvalue problem given in the lecture slides

$$\boldsymbol{S}_B \boldsymbol{w} = \lambda \boldsymbol{S}_W \boldsymbol{w} \qquad \text{where} \qquad \lambda := \frac{\boldsymbol{w}^\top \boldsymbol{S}_B \boldsymbol{w}}{\boldsymbol{w}^\top \boldsymbol{S}_W \boldsymbol{w}}.$$