

## Principal Component Analysis

Task 1. In this task, we will once again work with the MNIST training set as provided on Moodle. Choose three digit classes, e.g. 1, 2 and 3 and load  $N=1000$  images from each of the classes to the workspace. Store the data in a floating point matrix  $X$  of shape  $(784, 3*N)$  normalized to the number range  $[0, 1]$ . Furthermore, generate a color label matrix  $C$  of dimensions  $(3*N, 3)$ . Each row of  $C$  assigns an RGB color vector to the respective column of  $X$  as an indicator of the digit class. Choose  $[0, 0, 1]$ ,  $[0, 1, 0]$  and  $[1, 0, 0]$  for the three digit classes.

- Compute the row-wise mean  $\mu$  of  $X$  and subtract it from each column of  $X$ . Save the results as  $X\_c$ .
- Use `np.linalg.svd` with `full_matrices=False` to compute the singular value decomposition  $[U, \text{Sigma}, VT]$  of  $X\_c$ . Make sure the matrices are sorted in descending order with respect to the singular values.
- Use `reshape` in order to convert  $\mu$  and the first three columns of  $U$  to  $(28, 28)$ -matrices. Plot the resulting images. What do you see?
- Compute the matrix  $S = \text{np.dot}(\text{np.diag}(\text{Sigma}), VT)$ . Note that this yields the same result as  $S = \text{np.dot}(U.T, X\_c)$ . The  $S$  matrix contains the  $3*N$  scores for the principal components 1 to 784. Create a 2D scatter plot with  $C$  as its color parameter in order to plot the scores for the first *two* principal components of the data.

Task 2. In this task, we consider the problem of choosing the number of principal vectors. Assuming that  $\mathbf{X} \in \mathbb{R}^{p \times N}$  is the centered data matrix and  $\mathbf{P} = \mathbf{U}_k \mathbf{U}_k^\top$  is the projector onto the  $k$ -dimensional principal subspace, the dimension  $k$  is chosen such that the fraction of overall energy contained in the projection error does not exceed  $\epsilon$ , i.e.

$$\frac{\|\mathbf{X} - \mathbf{P}\mathbf{X}\|_F^2}{\|\mathbf{X}\|_F^2} = \frac{\sum_{i=1}^M \|\mathbf{x}_i - \mathbf{P}\mathbf{x}_i\|^2}{\sum_{i=1}^N \|\mathbf{x}_i\|^2} \leq \epsilon,$$

where  $\epsilon$  is usually chosen to be between 0.01 and 0.2.

The MIT VisTex database as provided on Moodle consists of a set of 167 RGB texture images of sizes  $(512, 512, 3)$ . Download the ZIP file, unpack it and make yourself familiar with the directory structure.

- a) After preprocessing the entire image set (converting to normalized grayscale matrices), divide the images into non overlapping tiles of sizes  $(64, 64)$  and create a centered data matrix  $X_c$  of size  $(p, N)$  from them, where  $p=64*64$  and  $N=167*(512/64)*(512/64)$ .
- b) Compute the SVD of  $X_c$  and make sure the singular values are sorted in descending order.
- c) Plot the fraction of signal energy contained in the projection error<sup>1</sup> for the principal subspace dimensions 0 to  $p$ . How many principal vectors do you need to retain 80%, 90%, 95% or 99% of the original signal energy?
- d) Discuss: Can you imagine a scenario, where signal energy is a bad measure of useful information?

## Helpful Python/Numpy functions

```
import imageio          contains imread
import matplotlib.pyplot contains plotting functionalities
```

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<sup>1</sup>Note that you do not need to evaluate any norms or projections. All you need is the result of subtask b)