

LAB3: Dimensionality Reduction

Goal: to study the problem of dimensionality reduction through Principal Component Analysis (PCA) and feature selection through Orthogonal Matching Pursuit (OMP) for a synthetic dataset.

This lab is divided into two parts depending of their level of complexity (**Beginner, Advanced**). Your goal is to complete entirely, at least, one of the two parts. Please note that a different notation can be used in the code as we used in the lectures.

PART I: Beginner

Warm up: Data Generation

Generate a 2-class dataset of D-dimensional points with N points for each class. Start with N = 100 and D = 30 and create a train and a test set.

1. The first two variables (dimensions) for each point will be generated by `MixGauss.py`, i.e., extracted from two Gaussian distributions, with centroids (1, 1) and (-1,-1) and `sigmas = 0.7` (the first one with `Y=1`, the second with `Y=-1`). Adjust the output labels of the classes to be {1,-1} respectively, e.g. using

```
Ytr[Y2tr==0] = 1.
```

To visualise the data: `plt.scatter(Xtr[:,0], Xtr[:,1], 25, Ytr)`

```
plt.show()
```

2. The remaining (D-2) variables will be generated by Gaussian noise with `sigma_noise = 0.01`, e.g.,

```
X2tr = normal(0, sigma_noise, size=(2*N, D-2))
```

```
X2ts = normal(0, sigma_noise, size=(2*N, D-2))
```

3. The final train and test data matrices will be composed as:

```
Xtr = np.concatenate((Xtr, X2tr, axis=1)
```

Principal Component Analysis

4. Compute the principal components of the training set, using the provided class `PCA.py`, i.e.

```
V, d, X_proj = PCA(Xtr, k)
```

Plot the first component of `X_proj`, the first 2 and the first 3 components. Reason on the meaning of the obtained plots and results. What is the effective dimensionality of this dataset?

5. Visualise/display the square root of the first $k=10$ eigenvalues, and the coefficients (eigenvectors) associated with the largest eigenvalue, i.e.,

```
plt.plot(range(10), np.sqrt(d))
plt.show()
plt.scatter(range(D), np.abs(V[:,i]))
plt.show()
```

Same for the second and third largest.

6. Repeat the above steps with a dataset generated using different `sigma_noise` in $\{0, 0.01, 0.1, 0.5, 0.7, 1:0.2:2\}$. To what extent is data visualisation by PCA affected by noise?

Variable Selection

7. Standardize the data matrix, so that each column has mean 0 and standard deviation 1. Use the statistics from the train set `Xtr` (mean and standard deviation) to standardize the corresponding test set `Xts`. Useful commands:

```
mean = np.mean(Xtr, axis=0) % mean of each column
std = np.std(Xtr, axis=0, ddof=1) % standard deviation
```

```
Xtr -= mean % remove mean of each column/dimension
```

```
Xtr = Xtr/std % scale std in each dimension for data point
```

8. Use the orthogonal matching pursuit algorithm, implemented in the class `OMatchingPursuit.py`, using `T` repetitions, to obtain `T-1` coefficients for a sparse approximation of the training set `Xtr`. Plot the resulting coefficients `w` using

```
plt.stem(range(D), w)
plt.xlim([-1, D])
plt.show()
```

What is the output when setting $T = 3$ and what is the interpretation of the indices of these first active dimensions (coefficients)?

9. Check the predicted labels on the training (and test) set when approximating the output using `w`:

```
Ypred = np.sign(np.dot(Xts, w))
error.append(calcErr(Y2ts, Ypred))
```

How does the train and test error change with the number of iterations of the method? Plot the errors on the same plot for increasing `T`.

1. By applying cross-validation on the training set through the provided `holdoutCVOMP.py` find the optimum number of iterations in the range `intIter = 2:D`

(indicative values: $\text{perc} = 0.5$, $\text{nr ip} = 30$).

$\text{it, Vm, Vs, Tm, Ts} = \text{holdoutCVOMP}(\text{Xtr, Y2tr, } 0.5, 5, \text{intIter})$

Plot the training and validation error on the same plot. What is the behaviour of the training and the validation errors with respect to the number of iterations?

PART II: Advanced

Compare the results of previous parts and evaluate the benefits of the two different methods for dimensionality reduction and feature selection when choosing $N \gg D$, $N \sim D$ and $N \ll D$.