

Problem Set 6

This homework you implement 3 algorithms. ISOMAP, PCA and MDS

Your code must be all written within the file HW6.py provided to you. The drawing part is also provided in the file.

Part 1 (5 points) Implement ISOMAP

Implement the classical MDS algorithm.

This algorithm takes as input a distance matrix $D = \{d_{ij}\}$ (k by k matrix) and number of component $d < n$ and returns a collection of points $\{y_i\}_{i=1}^k$ in the space R^d . The steps of the algorithm are given as follows:

- 1-Construct the matrix of squares of the distances $P^{(2)} = [d_{ij}^2]$.
2. Apply the double centering: $B = -\frac{1}{2}JP^{(2)}J$ where $J = I - \frac{1}{n}11'$, where n is the number of elements. The definition of 1 and $1'$ can be found in the lecture (see the example in the lecture).
3. Extract the largest d positive eigenvalues $\lambda_1 \dots \lambda_d$ of B and the corresponding m eigenvectors $e_1 \dots e_d$.
4. Construct the matrix $X = E_d \Lambda_d^{\frac{1}{2}}$, where E_d is the matrix of d eigenvectors and Λ_d is the diagonal matrix of d eigenvalues of B , respectively

An example of the above steps is given in the lecture so you may refer back to the lecture and use the example as a guide when you do the above implementation.

Note 1: you will need to use an eigensolver for to do step 3 in the above algorithm. One common choice is [here](#). Also, you can use the following [function](#) to do step 2.

Note 2. Use the data set given in this example [here](#) as a testing data set. Use $d=2$ when do the testing.

Part 2 (4 points) Implement ISOMAP and MDS

Just like the previous algorithm, this algorithm takes as input a collection of points $\mathbf{X}=\{x_i\}_{i=1}^k$ in R^n and number of component $d < n$, and the number of K nearest neighbors in the K -NN graph and returns a collection of points $\{y_i\}_{i=1}^k$ that represent the points $\{x_i\}_{i=1}^k$ in the space R^d . The steps of the algorithm are given as follows:

- 1- Construct the neighborhood graph of the data \mathbf{X} using the *K-NN neighborhood* graph we studied earlier in the course.
- 2- Use the Dijkstra algorithm or the Floyd–Warshall algorithm to find the distance between nodes on the graph.
- 3- Apply MDS on the distance matrix above and extract the coordinates with the desired dimension (part one of the algorithm). In step 1 and 2 you may use the function in sklearn and networkx that we have utilized before in earlier homeworks.

Note 2. Use the data set given in this example [here](#) as a testing data set. Use $d=2$ when do the testing. Use $K=10$.

Part 3 (3 points) Compare your results with the results in [here](#)

The following code imports a points cloud with the shape “S” that we studied many times during the lecture :

```
import matplotlib.pyplot as plt
from mpl_toolkits.mplot3d import Axes3D
from matplotlib.ticker import NullFormatter

from sklearn import manifold, datasets
```

```

# Next line to silence pyflakes. This import is needed.
Axes3D

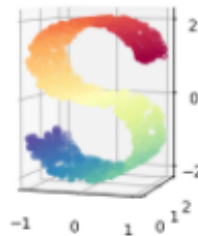
n_points = 1000
X, color = datasets.samples_generator.make_s_curve(n_points, random_state=0)
n_neighbors = 10
n_components = 2

fig = plt.figure(figsize=(15, 8))
plt.suptitle("Manifold Learning with %i points, %i neighbors"
             % (1000, n_neighbors), fontsize=14)

ax = fig.add_subplot(251, projection='3d')
ax.scatter(X[:, 0], X[:, 1], X[:, 2], c=color, cmap=plt.cm.Spectral)

```

It will also plot the data X for you.



Use the data X above as input for your MDS and ISOMAP functions and compare your results to the results obtained in the sklearn example [here](#).

Remark : MDS takes as input the distance matrix of X and not X itself so make sure you pass the distance matrix of X instead of X itself when you do your computation in this example.

Part 4 (3 points) PCA

Use PCA to reduce the dimension of the data set “S” to 2 dimension. Plot the result point cloud and explain your observation. (does PCA do a good job here ? why ?)

[PCA](#) can be found.