A Mathematical Introduction to Data Science **March 20, 2023**

Homework 6. Manifold Learning

Instructor: Yuan Yao *Due: 2 weeks later*

The problem below marked by * is optional with bonus credits.

1. *Order the faces:* The following dataset contains 33 faces of the same person ($Y \in \mathbb{R}^{112\times 92\times 33}$) in different angles,

   `https://yao-lab.github.io/data/face.mat`

   You may create a data matrix $X \in \mathbb{R}^{n\times p}$ where $n = 33, p = 112 \times 92 = 10304$ (e.g. `X=reshape(Y,[10304,33])';` in matlab).

   (a) Explore the MDS-embedding of the 33 faces on top two eigenvectors: order the faces according to the top 1st eigenvector and visualize your results with figures.

   (b) Explore the ISOMAP-embedding of the 33 faces on the $k = 5$ nearest neighbor graph and compare it against the MDS results. Note: you may try Tenenbaum's Matlab code `https://yao-lab.github.io/data/isomapII.m`

   (c) Explore the LLE-embedding of the 33 faces on the $k = 5$ nearest neighbor graph and compare it against ISOMAP. Note: you may try the following Matlab code `https://yao-lab.github.io/data/lle.m`

2. *Manifold Learning*: The following codes by Todd Wittman contain major manifold learning algorithms talked on class.

   `http://math.stanford.edu/~yuany/course/data/mani.m`

   Precisely, eight algorithms are implemented in the codes: MDS, PCA, ISOMAP, LLE, Hessian Eigenmap, Laplacian Eigenmap, Diffusion Map, and LTSA. The following nine examples are given to compare these methods,

   (a) Swiss roll;

   (b) Swiss hole;

   (c) Corner Planes;

   (d) Punctured Sphere;

   (e) Twin Peaks;

   (f) 3D Clusters;

   (g) Toroidal Helix;

   (h) Gaussian;

   (i) Occluded Disks.

Run the codes for each of the nine examples, and analyze the phenomena you observed.

*Moreover if possible, play with t-SNE using scikit-learn manifold package:

`http://scikit-learn.org/stable/modules/generated/sklearn.manifold.TSNE.html`

or any other implementations collected at

`http://lvdmaaten.github.io/tsne/`

3. *Nyström method:* In class, we have shown that every manifold learning algorithm can be regarded as Kernel PCA on graphs: (1) given N data points, define a neighborhood graph with N nodes for data points; (2) construct a positive semidefinite kernel K; (3) pursue spectral decomposition of K to find the embedding (using top or bottom eigenvectors). However, this approach might suffer from the expensive computational cost in spectral decomposition of K if N is large and K is non-sparse, e.g. ISOMAP and MDS.

   To overcome this hurdle, Nyström method leads us to a scalable approach to compute eigenvectors of low rank matrices. Suppose that an N-by-N positive semidefinite matrix $K \succeq 0$ admits the following block partition

$$K = \begin{bmatrix} A & B \\ B^T & C \end{bmatrix}. \tag{1}$$

   where A is an n-by-n block. Assume that A has the spectral decomposition $A = U\Lambda U^T$, $\Lambda = \mathrm{diag}(\lambda_i)$ ($\lambda_1 \geq \lambda_2 \geq \ldots \lambda_k > \lambda_{k+1} = \ldots = 0$) and $U = [u_1, \ldots, u_n]$ satisfies $U^T U = I$.

   (a) Assume that $K = XX^T$ for some $X = [X_1; X_2] \in \mathbb{R}^{N\times k}$ with the block $X_1 \in \mathbb{R}^{n\times k}$. Show that X_1 and X_2 can be decided by:

$$X_1 = U_k \Lambda_k^{1/2}, \tag{2}$$

$$X_2 = B^T U_k \Lambda_k^{-1/2}, \tag{3}$$

   where $U_k = [u_1, \ldots, u_k]$ consists of those k columns of U corresponding to top k eigenvalues λ_i ($i = 1, \ldots, k$).

   (b) Show that for general $K \succeq 0$, one can construct an approximation from (2) and (3),

$$\hat{K} = \begin{bmatrix} A & B \\ B^T & \hat{C} \end{bmatrix}. \tag{4}$$

   where $A = X_1 X_1^T$, $B = X_1 X_2^T$, and $\hat{C} = X_2 X_2^T = B^T A^\dagger B$, $A^\dagger$ denoting the Moore-Penrose (pseudo-) inverse of A. Therefore $\|\hat{K} - K\|_F = \|C - B^T A^\dagger B\|_F$. Here the matrix $C - B^T A^\dagger B =: K/A$ is called the (generalized) *Schur Complement* of A in K.

   (c) Explore Nyström method on the Swiss-Roll dataset (`http://yao-lab.github.io/data/swiss_roll_data.mat` contains 3D-data X; `http://yao-lab.github.io/data/swissroll.m` is the matlab code) with ISOMAP. To construct the block A, you may choose either of the following:

      n random data points;

*n landmarks as minimax k-centers (`https://yao-lab.github.io/data/kcenter.m`);

Some references can be found at:

[dVT04] Vin de Silva and J. B. Tenenbaum, "Sparse multidimensional scaling using landmark points", 2004, downloadable at `http://pages.pomona.edu/~vds04747/public/papers/landmarks.pdf`;

[P05] John C. Platt, "FastMap, MetricMap, and Landmark MDS are all Nyström Algorithms", 2005, downloadable at `http://research.microsoft.com/en-us/um/people/jplatt/nystrom2.pdf`.

(d) *Assume that A is invertible, show that

$$\det(K) = \det(A) \cdot \det(K/A),$$

(e) *Assume that A is invertible, show that

$$\mathrm{rank}(K) = \mathrm{rank}(A) + \mathrm{rank}(K/A).$$

(f) *Can you extend the identities in (c) and (d) to the case of noninvertible A? A good reference can be found at,

[Q81] Diane V. Quellette, "Schur Complements and Statistics", Linear Algebra and Its Applications, 36:187-295, 1981. `http://www.sciencedirect.com/science/article/pii/0024379581902329`