SOUTH UNIVERSITY OF SCIENCE AND TECHNOLOGY OF CHINA

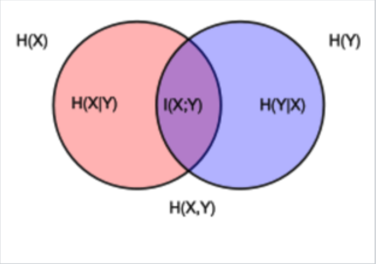
Intro to Big Data Science: Assignment 5

Due Date: May 20, 2025

✏ **Exercise 1** Recall the definition of information entropy, $H(P) = -\sum_{i=1}^{n} p_i \log p_i$, which means the maximal information contained in probability distribution P. Let X and Y be two random variables. The entropy $H(X,Y)$ for the joint distribution of (X,Y) is defined similarly. The conditional entropy is defined as:

$$\begin{aligned} H(X|Y) &= -\sum_{j} P(Y=y_j) H(X|Y=y_j) \\ &= -\sum_{j} P(Y=y_j)(\sum_{i} P(X=x_i|Y=y_j) \log P(X=x_i|Y=y_j)) \end{aligned}$$

1. Show that $H(X,Y) = H(X) + H(Y|X) = H(Y) + H(X|Y)$.
2. The mutual information (information gain) is defined as $I(X;Y) = H(X) - H(X|Y) = H(Y) - H(Y|X)$. Show that if X and Y are independent, then $I(X;Y) = 0$

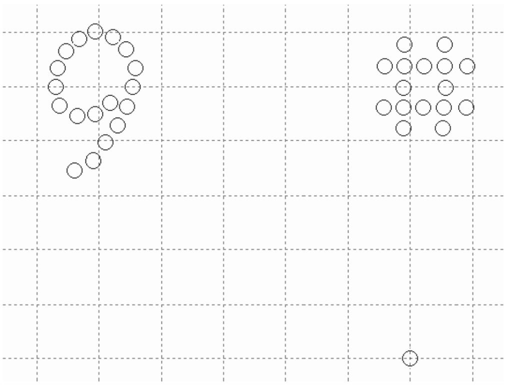


3. Define the Kullback-Leibler divergence as $D_{KL}(P\|Q) = -\sum_{i=1}^{n} p_i \log \frac{q_i}{p_i}$. Show that $I(X;Y) = D_{KL}(p(X,Y)\|p(X)p(Y))$.
4. (Optional) Furthermore, show that $D_{KL}(P\|Q) \geqslant 0$ for any P and Q by using Jensen's inequality. As a result, $I(X;Y) \geqslant 0$.

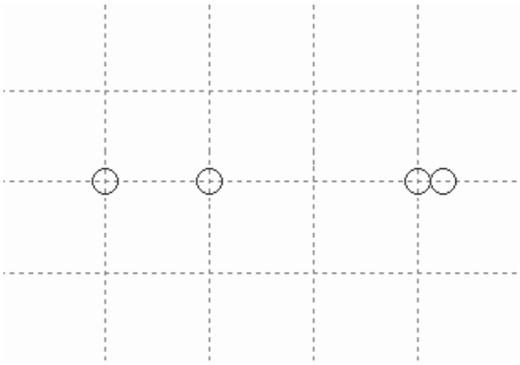
✏ **Problem 2** (Spectral Clustering)

1. We consider the 2-clustering problem, in which we have N data points $x_{1:N}$ to be grouped in two clusters, denoted by A and B. Given the N by N affinity matrix W (**Remember that in class we define the affinity matrix in the way that the diagonal entries are zero for undirected graphs**), consider the following two problems:

   - Min-cut: minimize $\sum\limits_{i\in A}\sum\limits_{j\in B} W_{ij}$;
   - Normalized cut: minimize $\frac{\sum_{i\in A}\sum_{j\in B} W_{ij}}{\sum_{i\in A}\sum_{j=1}^{N} W_{ij}} + \frac{\sum_{i\in A}\sum j\in B W_{ij}}{\sum_{i=1}^{N}\sum_{j\in B} W_{ij}}$.



(a)



(b)

   a) The data points are shown in Figure (a) above. The grid unit is 1. Let $W_{ij} = e^{-\|\mathbf{x}_i-\mathbf{x}_j\|_2^2}$, give the clustering results of min-cut and normalized cut respectively (Please draw a rough sketch and give the separation boundary in the answer book).

   b) The data points are shown in Figure (b) above. The grid unit is 1. Let $W_{ij} = e^{-\frac{\|\mathbf{x}_i-\mathbf{x}_j\|_2^2}{2\sigma^2}}$, describe the clustering results of min-cut algorithm for $\sigma^2 = 50$ and $\sigma^2 = 0.5$ respectively (Please draw a rough sketch and give the separation boundaries for each case of σ^2 in the answer book).

2. Now back to the setting of the 2-clustering problem shown in Figure (a). The grid unit is 1.

   a) If we use Euclidean distance to construct the affinity matrix W as follows:

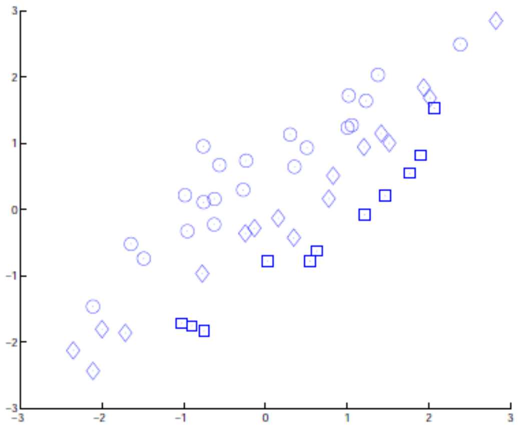
$$W_{ij} = \begin{cases} 1, & \text{if } \|\mathbf{x}_i - \mathbf{x}_j\|_2^2 \leqslant \sigma^2; \\ 0, & \text{otherwise.} \end{cases}$$

   What σ^2 value would you choose? Briefly explain.

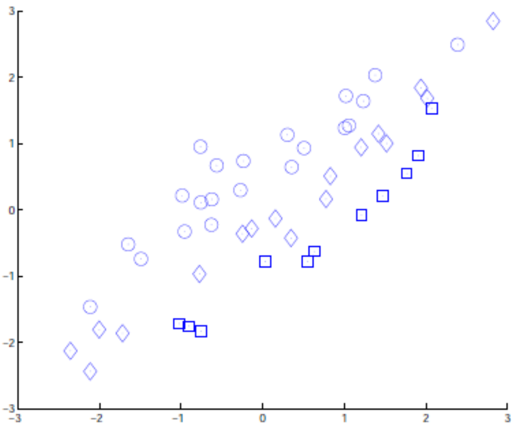
   b) The next step is to compute the first $k = 2$ dominant eigenvectors of the affinity matrix W. For the value of σ^2 you chose in the previous question, can you compute analytically the eigenvalues corresponding to the first two eigenvectors? If yes, compute and report the eigenvalues. If not, briefly explain.

✏ **Exercise 3** (Dimensionality Reduction)

1. (PCA vs. LDA) Plot the directions of the first PCA (plot (a)) and LDA (plot (b)) components in the following figures respectively.



(c) First PCA component



(d) First LDA component

2. (PCA and SVD) Given 6 data points in 5D space, $(1,1,1,0,0)$, $(-3,-3,-3,0,0)$, $(2,2,2,0,0)$, $(0,0,0,-1,-1)$, $(0,0,0,2,2)$, $(0,0,0,-1,-1)$. We can represent these data points by a 6×5 matrix $\mathbf{X}$, where each row corresponds to a data point:

$$\mathbf{X} = \begin{pmatrix} 1 & 1 & 1 & 0 & 0 \\ -3 & -3 & -3 & 0 & 0 \\ 2 & 2 & 2 & 0 & 0 \\ 0 & 0 & 0 & -1 & -1 \\ 0 & 0 & 0 & 2 & 2 \\ 0 & 0 & 0 & -1 & -1 \end{pmatrix}$$

a) What is the sample mean of the data set?

b) What is the SVD of the data matrix $\mathbf{X} = \mathbf{UDV}^T$, where $\mathbf{U}$ and $\mathbf{V}$ satisfy $\mathbf{U}^T\mathbf{U} = \mathbf{V}^T\mathbf{V} = \mathbf{I}_2$? Note that the SVD for this matrix must take the following form, where a, b, c, d, σ_1, σ_2 are the parameters you need to decide.

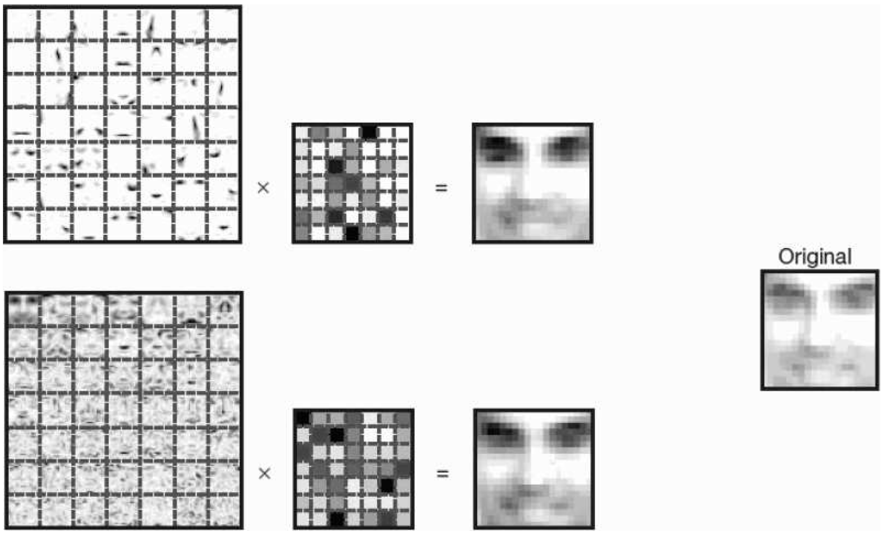
$$\mathbf{X} = \begin{pmatrix} a & 0 \\ -3a & 0 \\ 2a & 0 \\ 0 & b \\ 0 & -2b \\ 0 & b \end{pmatrix} \times \begin{pmatrix} \sigma_1 & 0 \\ 0 & \sigma_2 \end{pmatrix} \times \begin{pmatrix} c & c & c & 0 & 0 \\ 0 & 0 & 0 & d & d \end{pmatrix}$$

c) What is first principle component for the original data points?

d) If we want to project the original data points $\{\mathbf{x}_i\}_{i=1}^{6}$ into 1D space by principle component you choose, what is the sample variance of the projected data $\{\hat{\mathbf{x}}_i\}_{i=1}^{6}$?

e) For the projected data in d), now if we represent them in the original 5-d space, what is the reconstruction error $\frac{1}{6}\sum_{i=1}^{6}\|\mathbf{x}_i - \hat{\mathbf{x}}_i\|_2^2$?

3. The goal of Non-negative Matrix Factorization (NMF) is to reduce the dimensionality given non-negativity constraints. That is, we would like to find principle components $\mathbf{u}_1, \ldots, \mathbf{u}_r$, each of which is of dimension $d > r$, such that the d-dimensional data $\mathbf{x} \approx \sum_{i=1}^{r} z_i \mathbf{u}_i$, and all entries in $\mathbf{x}, \mathbf{z}, \mathbf{u}_{1:r}$ are non-negative. NMF tends to find sparse (usually small L_1 norm) basis vectors $\mathbf{u}_i$'s. Below is an example of applying PCA and NMF on a face image. Please point out the basis vectors in the equations and give them correct labels (NMF or PCA).



✏ **Exercise 4**(PCA as factor analysis and SVD)

PCA of a set of data in $\mathbb{R}^p$ provide a sequence of best linear approximations to those data, of all ranks $q \leqslant p$. Denote the observations by $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N$, and consider the rank-$q$ linear model for representing them

$$f(\alpha) = \mu + \mathbf{V}_q \alpha$$

where μ is a location vector in $\mathbb{R}^p$, V_q is a $p \times q$ matrix with q **orthogonal unit vectors** as columns, and α is a q vector of parameters. If we can find such a model, then we can reconstruct each $\mathbf{x}_i$ by a low dimensional coordinate vector α_i through

$$\mathbf{x}_i = f(\alpha_i) + \epsilon_i = \mu + \mathbf{V}_q \alpha_i + \epsilon_i \qquad (1)$$

where $\epsilon_i \in \mathbb{R}^p$ are noise terms. Then PCA amounts to minimizing this reconstruction error by least square method

$$\min_{\mu,\{\alpha_i\},\mathbf{V}_q} \sum_{i=1}^{N} \|\mathbf{x}_i - \mu - \mathbf{V}_q \alpha_i\|^2$$

1. Assume $\mathbf{V}_q$ is known and treat μ and α_i as unknowns. Show that the least square problem

   $$\min_{\mu,\{\alpha_i\}} \sum_{i=1}^{N} \|\mathbf{x}_i - \mu - \mathbf{V}_q \alpha_i\|^2$$

   is minimized by

   $$\hat{\mu} = \bar{\mathbf{x}} = \frac{1}{N}\sum_{i=1}^{N} \mathbf{x}_i, \tag{2}$$

   $$\hat{\alpha}_i = \mathbf{V}_q^T(\mathbf{x}_i - \bar{\mathbf{x}}). \tag{3}$$

   Also show that the solution for $\hat{\mu}$ is not unique. Give a family of solutions for $\hat{\mu}$.

2. For the standard solution (2), we are left with solving

   $$\min_{\mathbf{V}_q} \sum_{i=1}^{N} \|(\mathbf{x}_i - \bar{\mathbf{x}}) - \mathbf{V}_q\mathbf{V}_q^T(\mathbf{x}_i - \bar{\mathbf{x}})\|^2 = \min_{\mathbf{V}_q} \mathrm{Tr}\Big(\tilde{\mathbf{X}}(\mathbf{I}_p - \mathbf{V}_q\mathbf{V}_q^T)\tilde{\mathbf{X}}^T\Big). \tag{4}$$

   Here we introduce the centered sample matrix

   $$\tilde{\mathbf{X}} = (\mathbf{I}_N - \frac{1}{N}\mathbf{J}_N)\mathbf{X} = \begin{pmatrix} (\mathbf{x}_1 - \bar{\mathbf{x}})^T \\ \vdots \\ (\mathbf{x}_N - \bar{\mathbf{x}})^T \end{pmatrix} \in \mathbb{R}^{N\times p}$$

   where $\mathbf{I}_N$ is $N \times N$ identity matrix and $\mathbf{J}_N$ is a matrix whose entries are all 1's. Recall the singular value decomposition (SVD) in linear algebra: $\tilde{\mathbf{X}} = \mathbf{U}\mathbf{D}\mathbf{V}^T$. Here $\mathbf{U}$ is an $N \times p$ orthogonal matrix ($\mathbf{U}^T\mathbf{U} = \mathbf{I}_p$) whose columns $\mathbf{u}_j$ are called the left singular vectors; $\mathbf{V}$ is a $p \times p$ orthogonal matrix ($\mathbf{V}^T\mathbf{V} = \mathbf{I}_p$) with columns $\mathbf{v}_j$ called the right singular vectors, and $\mathbf{D}$ is a $p \times p$ diagonal matrix, with diagonal elements $d_1 \geqslant d_2 \geqslant \cdots \geqslant d_p \geqslant 0$ known as the singular values.

   Show that the solution $\mathbf{V}_q$ to problem (4) consists of the first q columns of $\mathbf{V}$. (Then the optimal $\hat{\alpha}_i$ are given by the i-th row with the first q columns of $\mathbf{UD}$.)

Remark: The model (1), in general, gives the factor analysis in multivariate statistics:

$$\mathbf{x} = \mu + \mathbf{V}_q \alpha + \epsilon$$

In traditional factor analysis, α_j with $j = 1, \ldots, q$ is assumed to be Gaussian and uncorrelated as well as ϵ_i with $i = 1, \ldots, p$. However, Independent Component Analysis (ICA) instead assumes α_j with $j = 1, \ldots, q$ is assumed to be non-Gaussian and independent. Because of the independence, ICA is particularly useful in separating mixed signals.

✎ **Exercise 5 (idatacourse.cn)** Online study and exercises.

✎ **Exercise 6 (idatacoding.cn)** This is the project that you need to finish via the online system. There are two projects: one is about credit risk analysis via classification (“个人信用风险评估”), this is a mandatory project; the other is weibo data analysis (“微博数据舆情分析”) which may need the knowledge of deep learning (optional). Basically, we will ask you to finish the first project. But if you want, you can try the second one. The deadline for this project is **June 6, 2025**.