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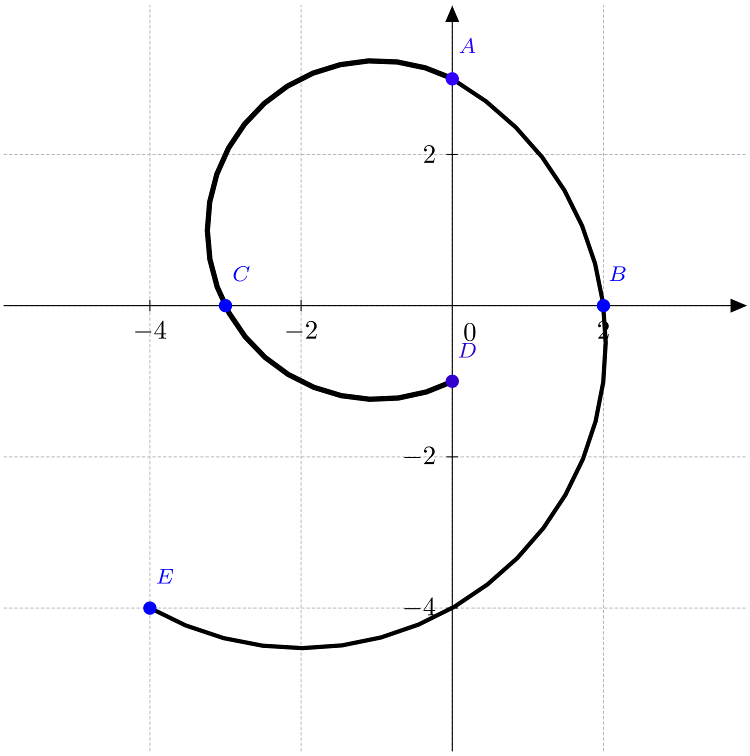
Exercise 8

Friday, December 7, 2018

Problem 1. *(Isomap)* In this exercise, we examine what happens if the dataset is not large enough to find its geometry. Consider five vectors $\mathbf{A}, \mathbf{B}, \mathbf{C}, \mathbf{D}$ and $\mathbf{E}$ given as follows



$$\mathbf{A} = \begin{pmatrix} 0 \\ 3 \end{pmatrix}, \mathbf{B} = \begin{pmatrix} 2 \\ 0 \end{pmatrix}, \mathbf{C} = \begin{pmatrix} -3 \\ 0 \end{pmatrix}, \mathbf{D} = \begin{pmatrix} 0 \\ -1 \end{pmatrix}, \mathbf{E} = \begin{pmatrix} -4 \\ 4 \end{pmatrix}.$$

a) Construct the graph for the Isomap based on 1-nearest neighbor and 2-nearest neighbor criteria and the mutual distances as the weights. Estimate the geodesic distance of $\mathbf{E}$ and $\mathbf{D}$.

b) Construct the graph for the Isomap using an ϵ. Discuss the choice of ϵ.

Problem 2. *(Diffusion Map)*

Suppose that a dataset is composed of n real vectors $\mathbf{x}_i$ for $i = 1, 2, \ldots, n$, of dimension m ($\mathbf{x}_i \in \mathbb{R}^m$).

a) In a diffusion map, which properties must be satisfied by kernel functions?

b) Could the following functions be used as valid kernel functions for diffusion maps? Please give a reason for your answer (one phrase per function is enough).

- $K_1(\mathbf{x}_i, \mathbf{x}_j) = \|\mathbf{x}_j - \mathbf{x}_i\|_2^2$,
- $K_2(\mathbf{x}_i, \mathbf{x}_j) = 1 - \|\mathbf{x}_j - \mathbf{x}_i\|_2$,
- $K_3(\mathbf{x}_i, \mathbf{x}_j) = \cos(\frac{\pi}{2}\|\mathbf{x}_j - \mathbf{x}_i\|_2)$ for $\|\mathbf{x}_j - \mathbf{x}_i\|_2 \leq 1$, and zero elsewhere,
- $K_4(\mathbf{x}_i, \mathbf{x}_j) = \max\{1 - (\|\mathbf{x}_j\|_2^2 - \mathbf{x}_j^{\mathrm{T}}\mathbf{x}_i), 0\}$.

Let the dataset be composed of the following 3 vectors ($n = 3$) of dimension 3 ($m = 3$)

$$\mathbf{x}_1^{\mathrm{T}} = \begin{pmatrix} 1 & -1 & 1 \end{pmatrix}, \qquad \mathbf{x}_2^{\mathrm{T}} = \begin{pmatrix} -1 & -1 & -1 \end{pmatrix}, \qquad \mathbf{x}_3^{\mathrm{T}} = \begin{pmatrix} -1 & 1 & -1 \end{pmatrix},$$

and the kernel function be given by $K(\mathbf{x}_i, \mathbf{x}_j) = \max\{1 - \frac{1}{6}\|\mathbf{x}_j - \mathbf{x}_i\|_2^2, 0\}$.

c) For the random walk of the diffusion map, a weight matrix $\mathbf{W}$ is needed. Calculate the remaining weights of the following weight matrix $\mathbf{W} \in \mathbb{R}^{3\times 3}$:

$$\mathbf{W} = \begin{bmatrix} 1 & w_{12} & 0 \\ w_{21} & 1 & w_{23} \\ 0 & w_{32} & 1 \end{bmatrix}$$

d) In another application with $n = 3$, the values of $\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3$ lead to the following decomposition of the transition matrix $\mathbf{M}$:

$$\mathbf{M} = \begin{bmatrix} 1 & 0 & 1 \\ 0 & \sqrt{2} & 0 \\ 1 & 0 & -1 \end{bmatrix} \begin{bmatrix} 3 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 1 \\ 0 & \sqrt{2} & 0 \\ 1 & 0 & -1 \end{bmatrix}^{\mathrm{T}}$$

The left and right eigenvectors of $\mathbf{M}$ are denoted as $\boldsymbol{\phi}_i$ and $\boldsymbol{\psi}_i$ for $i = 1, 2, 3$. The transition matrix $\mathbf{M}$ can be expressed as $\mathbf{M} = \sum_{k=1}^{3} \lambda_k \boldsymbol{\phi}_k \boldsymbol{\psi}_k^{\mathrm{T}}$. What are the values of λ_k for $k = 1, 2, 3$?

Problem 3. *(Diffusion Distance)* Let $\mathbf{x}_1, \ldots, \mathbf{x}_n$ be some points in $\mathbb{R}^p$, and the garph $(V, E, \mathbf{W})$ is constructed based on those points using a kernel function. Transition probability matrix is constructed accordingly. Suppose that the diffusion map of a vertex v_i is given by $\boldsymbol{\phi}_t(v_i)$. For any pair of nodes v_i and v_j in the graph, prove:

$$\|\boldsymbol{\phi}_t(v_i) - \boldsymbol{\phi}_t(v_j)\|^2 = \sum_{l=1}^{n} \frac{1}{\deg(l)} \Big(\mathbb{P}(X_t = l | X_0 = i) - \mathbb{P}(X_t = l | X_0 = j)\Big)^2.$$