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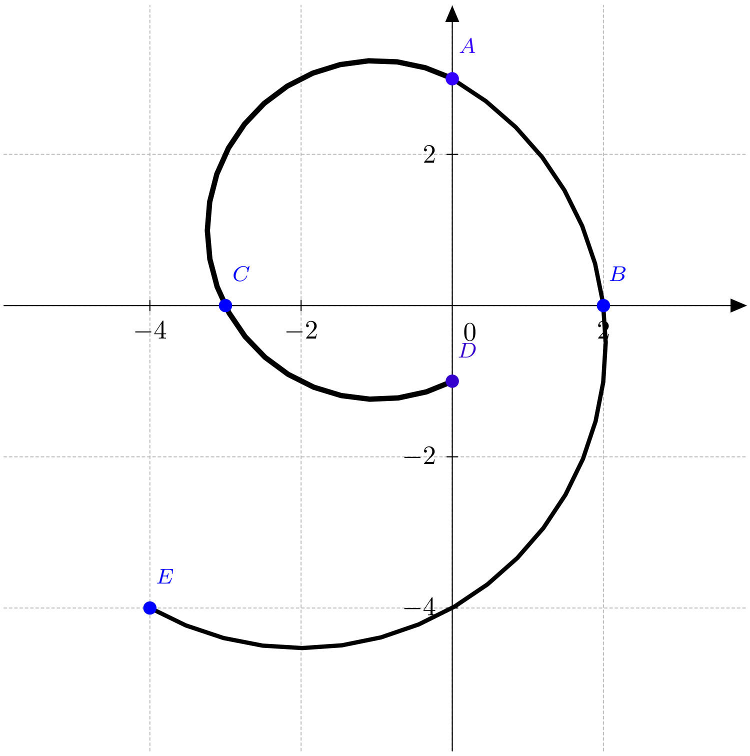
Exercise 8
- Proposed Solution -

Friday, December 7, 2018

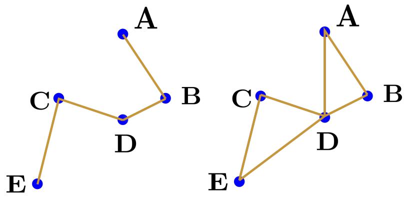
Solution of Problem 1

(Isomap) Consider five vectors $\mathbf{A}, \mathbf{B}, \mathbf{C}, \mathbf{D}$ and $\mathbf{E}$ given as follows



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

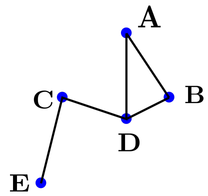
a) The following figure shows when 1NN and 2NN is used for graph construction. For



1NN graph $\delta(\mathbf{E}, \mathbf{D})$ is determined by a single path and is given by $\sqrt{10} + \sqrt{17}$. For 2NN graph, $\delta(\mathbf{E}, \mathbf{D})$ is the minimum of $\sqrt{32}$ and $\sqrt{10} + \sqrt{17}$, which is already known from triangle inequality, and it is $\sqrt{32}$. In both examples, it is clear that the geodesic estimation is wrong and particularly worse for 2NN.

b) The smallest distance is given by the distance of $\mathbf{D}$ and $\mathbf{B}$. Therefore for $\epsilon < \sqrt{5}$, the graph consists of isolated points.

For $\epsilon \in [\sqrt{5}, \sqrt{10})$, there is only a single edge between $\mathbf{D}$ and $\mathbf{B}$; for $\epsilon \in [\sqrt{10}, \sqrt{13})$ two edges appear between $\mathbf{D}, \mathbf{B}$ and $\mathbf{C}, \mathbf{D}$. The analysis go on accordingly. The graph becomes connect only if $\epsilon \geq \sqrt{17}$; for $\epsilon = \sqrt{17}$, the following graph is obtained. When ϵ



starts to go above 5 more edges appear and the graph becomes ultimately fully connected for $\epsilon > \sqrt{52}$.

Solution of Problem 2

(Diffusion Map)

a) A kernel function $K(\mathbf{x}_i, \mathbf{x}_j)$ of a diffusion map must follow the following properties:

- Symmetry: $K(\mathbf{x}_i, \mathbf{x}_j) = K(\mathbf{x}_j, \mathbf{x}_i)$,
- Non-negativity: $K(\mathbf{x}_i, \mathbf{x}_j) \geq 0$,
- Locality: If $\|\mathbf{x}_j - \mathbf{x}_i\|_2 \to \infty$ then $K(\mathbf{x}_i, \mathbf{x}_j) \to 0$. If $\|\mathbf{x}_j - \mathbf{x}_i\|_2 \to 0$ then $K(\mathbf{x}_i, \mathbf{x}_j) \to 1$.

b)

- $K_1(\mathbf{x}_i, \mathbf{x}_j) = \|\mathbf{x}_j - \mathbf{x}_i\|^2$: No, locality is violated.
- $K_2(\mathbf{x}_i, \mathbf{x}_j) = 1 - \|\mathbf{x}_j - \mathbf{x}_i\|_2$: No, non-negativity and locality are violated.
- $K_3(\mathbf{x}_i, \mathbf{x}_j) = \cos(\frac{\pi}{2}\|\mathbf{x}_j - \mathbf{x}_i\|_2)$ for $\|\mathbf{x}_j - \mathbf{x}_i\|_2 \leq 1$, and zero elsewhere: : Yes, this could be a kernel function.
- $K_4(\mathbf{x}_i, \mathbf{x}_j) = \max\{1 - (\|\mathbf{x}_j\|_2^2 - \mathbf{x}_j^{\mathrm{T}}\mathbf{x}_i), 0\}$: No, symmetry is violated.

c)

$$\mathbf{W} = \begin{bmatrix} K(\mathbf{x}_1, \mathbf{x}_1) & K(\mathbf{x}_1, \mathbf{x}_2) & K(\mathbf{x}_1, \mathbf{x}_3) \\ K(\mathbf{x}_2, \mathbf{x}_1) & K(\mathbf{x}_2, \mathbf{x}_2) & K(\mathbf{x}_2, \mathbf{x}_3) \\ K(\mathbf{x}_3, \mathbf{x}_1) & K(\mathbf{x}_3, \mathbf{x}_2) & K(\mathbf{x}_3, \mathbf{x}_3) \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & \frac{1}{3} \\ 0 & \frac{1}{3} & 1 \end{bmatrix}.$$

d) We know that $\mathbf{M}$ can be decomposed as $\mathbf{M} = \mathbf{\Phi}\mathbf{\Delta}\mathbf{\Psi}^{\mathrm{T}}$, where $\mathbf{\Phi}$ and $\mathbf{\Psi}$ are bi-orthogonal (i.e., $\mathbf{\Phi}^{\mathrm{T}}\mathbf{\Psi} = \mathbf{I}_3$). We observe that the provided expression follows the same form, sicne the columns corresponding to the left and right eigenvectors of $\mathbf{M}$ are orthogonal. Nevertheless, these columns are not properly scaled since

$$\begin{bmatrix} 1 & 0 & 1 \\ 0 & \sqrt{2} & 0 \\ 1 & 0 & -1 \end{bmatrix}^{\mathrm{T}} \begin{bmatrix} 1 & 0 & 1 \\ 0 & \sqrt{2} & 0 \\ 1 & 0 & -1 \end{bmatrix} = \begin{bmatrix} 2 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{bmatrix} = 2\mathbf{I}_3$$

Therefore, by properly normalizing the provided relation we obtain $\mathbf{M} = \mathbf{\Phi}\mathbf{\Delta}\mathbf{\Psi}^{\mathrm{T}}$ as

$$\begin{aligned}\mathbf{M} &= \left(\frac{1}{\sqrt{2}}\begin{bmatrix}1 & 0 & 1\\ 0 & \sqrt{2} & 0\\ 1 & 0 & -1\end{bmatrix}\right)\left(2\begin{bmatrix}3 & 0 & 0\\ 0 & 2 & 0\\ 0 & 0 & 1\end{bmatrix}\right)\left(\frac{1}{\sqrt{2}}\begin{bmatrix}1 & 0 & 1\\ 0 & \sqrt{2} & 0\\ 1 & 0 & -1\end{bmatrix}\right)^{\mathrm{T}}\\ &= \mathbf{\Phi}\mathbf{\Delta}\mathbf{\Psi}^{\mathrm{T}}\end{aligned}$$

Therefore, since $\mathbf{\Delta} = \operatorname{diag}(\lambda_k)_{k=1,2,3}$, we have that $\lambda_1 = 6$, $\lambda_2 = 4$ and $\lambda_3 = 2$.

Solution of Problem 3

First of all, see that:

$$\begin{aligned}&\sum_{l=1}^{n}\frac{1}{\deg(l)}\Big(\mathbb{P}(X_t = l|X_0 = i) - \mathbb{P}(X_t = l|X_0 = j)\Big)^2\\ &\quad= \sum_{l=1}^{n}\frac{1}{\deg(l)}\left(\sum_{k=1}^{n}\lambda_k^t\phi_{k,i}\psi_{k,l} - \sum_{k=1}^{n}\lambda_k^t\phi_{k,j}\psi_{k,l}\right)^2 = \sum_{l=1}^{n}\frac{1}{\deg(l)}\left(\sum_{k=1}^{n}\lambda_k^t(\phi_{k,i}-\phi_{k,j})\psi_{k,l}\right)^2\\ &\quad= \sum_{l=1}^{n}\left(\sum_{k=1}^{n}\lambda_k^t(\phi_{k,i}-\phi_{k,j})\frac{\psi_{k,l}}{\sqrt{\deg(l)}}\right)^2 = \left\|\sum_{k=1}^{n}\lambda_k^t(\phi_{k,i}-\phi_{k,j})\mathbf{D}^{-1/2}\boldsymbol{\psi}_k\right\|^2\end{aligned}$$

Note that $\mathbf{D}^{-1/2}\mathbf{\Psi}$ is equal to $\mathbf{V}$, the eigenvalue matrix in spectral decomposition of $\mathbf{S}$. Therefore $\mathbf{D}^{-1/2}\boldsymbol{\psi}_k$'s are orthonormal, and we have:

$$\left\|\sum_{k=1}^{n}\lambda_k^t(\phi_{k,i}-\phi_{k,j})\mathbf{D}^{-1/2}\boldsymbol{\psi}_k\right\|^2 = \sum_{k=1}^{n}(\lambda_k^t)^2(\phi_{k,i}-\phi_{k,j})^2 = \sum_{k=1}^{n}(\lambda_k^t\phi_{k,i}-\lambda_k^t\phi_{k,j})^2 = \|\boldsymbol{\phi}_t(v_i)-\boldsymbol{\phi}_t(v_j)\|^2.$$