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Exercise 7
- Proposed Solution -

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Solution of Problem 1

(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 2

First of all, see that:

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

Note that $\mathbf{D}^{-1/2}\boldsymbol{\Psi}$ 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:

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

Solution of Problem 3

a) ***Forward direction***:

If the graph is disconnected, then the vertex set V can be partitioned into two sets A and B such that no edge exists between A and B. In the transition matrix $\mathbf{M}$, non-zero entries appear only on the entries inside $A\times A$ and $B\times B$. Let $\mathbf{M}_{C,D}$ is constructed as the submatrix of $\mathbf{M}$ by choosing rows from the set C and columns from the set D. Then $\mathbf{M}_{A,A}$ and $\mathbf{M}_{B,B}$ are both transition matrices on their own. Then $\boldsymbol{\chi}_A$ and $\boldsymbol{\chi}_B$ are both eigenvectors of those matrices with eigenvalues equal to one, where $\boldsymbol{\chi}_A=(\chi_A(i))_{1\le i\le n}$, with $\chi_A(x)=0$ if $x\notin A$ and $\chi_A(x)=1$ if $x\in A$. Therefore there are at least two eigenvalues equal to one in this case.

Reverse direction:

Suppose that there is more than one eigenvalue equal to one.

However, it is known that $|\lambda_k|\le 1$ for all eigenvalues of $\mathbf{M}$.

Let $\mathbf{m}=(m_1,\dots,m_n)^T$ be the eigenvector corresponding to $\lambda_2=1$. If $|m_l|=\max_{1\le j\le n}|m_j|$, we have:

$$|\lambda_2|\le\sum_{j=1}^{n}M_{lj}\frac{|m_j|}{|m_l|}\le\sum_{j=1}^{n}M_{lj}=1.$$

The equality obtains if $\frac{|m_j|}{|m_l|}=1$ for those j where $M_{lj}\neq 0$ and m_j's have those same sign. We can assume that $m_l=1$. Define the the set A as:

$$A=\{k:m_k=1\}.$$

Since the first eigenvector is $\mathbf{1}_n$, the second eigenvector should be different and hence $A \neq \{1, \dots, n\}$ and $A^c \neq \emptyset$. For each $k \in A$, we have:

$$\sum_{j=1}^{n} M_{kj} m_j = 1.$$

Note that $\sum_{j=1}^{n} M_{kj} = 1$ and $m_j < 1$ for $j \in A^c$. Therefore to have the equality, again $m_j = 1$ whenever $M_{kj} \neq 0$. In other words, $M_{ij} = 0$ for $j \in A^c$ and $i \in A$. Since $M_{ij} = \frac{w_{ij}}{\deg(i)}$, $M_{ji} = 0$ for $j \in A^c$ and $i \in A$. In other words there is no edge between the nodes of A and A^c. Hence the graph is disconnected.

Similar argument can be used by looking at m_k, $k \in A^c$. Since $M_{ki} = 0$ for $i \in A$, then $\sum_{j \in A^c} M_{kj} m_j = m_k$. Taking a k maximum absolute value entry and applying the same argument, another set B can be constructed having $m_j = m_k$ for $j \in B$ (this time we do not have $m_k = 1$). The set B represents another connected component of the graph. The process can be continued by removing the previous connected components from the graph and analysing again the remaining graph.

b) ***Forward direction***:

If the graph is bipartite, then the vertex set V can be partitioned into two sets A and B such that no edge exists inside A and inside B but only between them. In the transition matrix $\mathbf{M}$, non-zero entries appear only on the entries inside $A \times B$ and $B \times A$. Without loss of generality assume that $A = \{1, \dots, l\}$ and $B = \{l+1, \dots, n\}$. Then:

$$\mathbf{M} \begin{bmatrix} \mathbf{1}_A \\ \mathbf{0}_B \end{bmatrix} = \begin{bmatrix} \mathbf{0}_{A \times A} & \mathbf{M}_{A \times B} \\ \mathbf{M}_{B \times A} & \mathbf{0}_{B \times B} \end{bmatrix} \begin{bmatrix} \mathbf{1}_A \\ \mathbf{0}_B \end{bmatrix} = \begin{bmatrix} \mathbf{0}_A \\ \mathbf{1}_B \end{bmatrix}$$

$$\mathbf{M} \begin{bmatrix} \mathbf{0}_A \\ \mathbf{1}_B \end{bmatrix} = \begin{bmatrix} \mathbf{0}_{A \times A} & \mathbf{M}_{A \times B} \\ \mathbf{M}_{B \times A} & \mathbf{0}_{B \times B} \end{bmatrix} \begin{bmatrix} \mathbf{0}_A \\ \mathbf{1}_B \end{bmatrix} = \begin{bmatrix} \mathbf{1}_A \\ \mathbf{0}_B \end{bmatrix}$$

That implies:

$$\mathbf{M} \begin{bmatrix} \mathbf{1}_A \\ -\mathbf{1}_B \end{bmatrix} = \begin{bmatrix} -\mathbf{1}_A \\ \mathbf{1}_B \end{bmatrix}.$$

Therefore -1 is an eigenvalue.

Reverse direction:

Suppose that $\lambda_2 = -1$ is an eigenvalue. If $|m_l| = \max_{1 \leq j \leq n} |m_j|$, we have:

$$|\lambda| \leq \sum_{j=1}^{n} M_{lj} \frac{|m_j|}{|m_l|} \leq \sum_{j=1}^{n} M_{lj} = 1.$$

Since $\lambda = -1$, the equality obtains if $m_j = -m_l$ for those j where $M_{lj} \neq 0$. We can assume that $m_l = 1$. Define the the sets A_{-1}, A_1, A_0 as:

$$A_{-1} = \{k : m_k = -1\}, A_1 = \{k : m_k = 1\}, A_0 = \{k : |m_k| \neq 1\}.$$

For each $k \in A_{-1}$, we have:

$$\sum_{j=1}^{n} M_{kj} m_j = 1.$$

This means that if $k \in A_{-1}$, then $m_j = 1$ for $M_{kj} \neq 0$. In other words, if $m_j \neq 1$ then $M_{kj} = 0$, which is:

$$M_{kj} = 0 \text{ for } k \in A_{-1}, j \in A_1^c.$$

In other words no edge exists between the vertices inside A_{-1}, also there is no edge from A_{-1} to A_0. The edges from A_{-1} go only to A_1.

Similarly for each $k \in A_1$, we have:

$$\sum_{j=1}^{n} M_{kj} m_j = -1.$$

This means that if $k \in A_1$, then $m_j = -1$ for $M_{kj} \neq 0$. In other words, if $m_j \neq -1$ then $M_{kj} = 0$, which is:

$$M_{kj} = 0 \text{ for } k \in A_1, j \in A_{-1}^c.$$

In other words no edge exists between the vertices inside A_1, also there is no edge from A_1 to A_0. The edges from A_1 go only to A_{-1}.

This means that $A_1 \cup A_{-1}$ is a component which is bipartite and it is disconnected from A_0. Since it is assumed that the graph is connected, then $A_0 = \emptyset$.