Solution of Problem 1

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

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

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

1NN graph $\delta(E, D)$ is determined by a single path and is given by $\sqrt{10} + \sqrt{17}$. For 2NN graph, $\delta(E, D)$ 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 $D$ and $B$. 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 $D$ and $B$; for $\epsilon \in [\sqrt{10}, \sqrt{13})$ two edges appear between $D, B$ and $C, D$. 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 $\epsilon$ starts to go above 5 more edges appear and the graph becomes ultimately fully connected for $\epsilon > \sqrt{52}$.

\[ \begin{array}{c}
\text{Solution of Problem 2} \\
\text{(Diffusion Map)}
\end{array} \]

a) A kernel function $K(x_i, x_j)$ of a diffusion map must follow the following properties:

- Symmetry: $K(x_i, x_j) = K(x_j, x_i)$,
- Non-negativity: $K(x_i, x_j) \geq 0$,
- Locality: If $\|x_j - x_i\|_2 \to \infty$ then $K(x_i, x_j) \to 0$. If $\|x_j - x_i\|_2 \to 0$ then $K(x_i, x_j) \to 1$.

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

c) $W = \begin{bmatrix} K(x_1, x_1) & K(x_1, x_2) & K(x_1, x_3) \\ K(x_2, x_1) & K(x_2, x_2) & K(x_2, x_3) \\ K(x_3, x_1) & K(x_3, x_2) & K(x_3, x_3) \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & \frac{1}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{2}} & 1 \end{bmatrix}.$

d) We know that $M$ can be decomposed as $M = \Phi \Delta \Psi^T$, where $\Phi$ and $\Psi$ are bi-orthogonal (i.e., $\Phi^T \Psi = I_3$). We observe that the provided expression follows the same form, since the columns corresponding to the left and right eigenvectors of $M$ are orthogonal. Nevertheless, these columns are not properly scaled since

\[ \begin{bmatrix}1 & 0 & 1 \\ 0 & \sqrt{2} & 0 \\ 1 & 0 & -1 \end{bmatrix}^T \begin{bmatrix}1 & 0 & 1 \\ 0 & \sqrt{2} & 0 \\ 1 & 0 & -1 \end{bmatrix} = \begin{bmatrix}2 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{bmatrix} = 2I_3 \]
Therefore, by properly normalizing the provided relation we obtain $M = \Phi \Delta \Psi^T$ as

$$M = \left( \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 0 & 1 \\ 0 & \sqrt{2} & 0 \\ 1 & 0 & -1 \end{bmatrix} \right) \left( 2 \begin{bmatrix} 3 & 0 & 0 \end{bmatrix} \right) \left( \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 0 & 1 \\ 0 & \sqrt{2} & 0 \\ 1 & 0 & -1 \end{bmatrix} \right)^T$$

$$= \Phi \Delta \Psi^T$$

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

**Solution of Problem 3**

First of all, see that:

$$\sum_{l=1}^{n} \frac{1}{\deg(l)} \left( \mathbb{P}(X_t = l|X_0 = i) - \mathbb{P}(X_t = l|X_0 = j) \right)^2$$

$$= \sum_{l=1}^{n} \frac{1}{\deg(l)} \left( \sum_{k=1}^{n} \lambda_k^l \phi_{k,i} \psi_{k,l} - \sum_{k=1}^{n} \lambda_k^l \phi_{k,j} \psi_{k,l} \right)^2 = \sum_{l=1}^{n} \frac{1}{\deg(l)} \left( \sum_{k=1}^{n} \lambda_k^l (\phi_{k,i} - \phi_{k,j}) \psi_{k,l} \right)^2$$

$$= \sum_{l=1}^{n} \left( \sum_{k=1}^{n} \lambda_k^l (\phi_{k,i} - \phi_{k,j}) \frac{\psi_{k,l}}{\sqrt{\deg(l)}} \right)^2 = \left\| \sum_{k=1}^{n} \lambda_k^l (\phi_{k,i} - \phi_{k,j}) \mathbf{D}^{-1/2} \psi_k \right\|^2$$

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

$$\left\| \sum_{k=1}^{n} \lambda_k^l (\phi_{k,i} - \phi_{k,j}) \mathbf{D}^{-1/2} \psi_k \right\|^2 = \sum_{k=1}^{n} (\lambda_k^l)^2 (\phi_{k,i} - \phi_{k,j})^2 = \sum_{k=1}^{n} (\lambda_k^l \phi_{k,i} - \lambda_k^l \phi_{k,j})^2 = \| \phi_t(v_i) - \phi_t(v_j) \|^2.$$