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Exercise 6
- Proposed Solution -

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Solution of Problem 1

a) First of all, note that:

$$\overline{\mathbf{x}} = \frac{1}{n}\mathbf{X}\mathbf{1}_n.$$

Moreover:

$$\mathbf{S}_n = \frac{1}{n-1}(\mathbf{X} - \overline{\mathbf{x}}\mathbf{1}_n^T)(\mathbf{X} - \overline{\mathbf{x}}\mathbf{1}_n^T)^T.$$

Therefore:

$$\mathbf{S}_n = \frac{1}{n-1}(\mathbf{X} - \frac{1}{n}\mathbf{X}\mathbf{1}_n\mathbf{1}_n^T)(\mathbf{X} - \frac{1}{n}\mathbf{X}\mathbf{1}_n\mathbf{1}_n^T)^T = \frac{1}{n-1}\mathbf{X}\mathbf{E}_n\mathbf{E}_n^T\mathbf{X}^T.$$

Using $\mathbf{E}_n\mathbf{E}_n = \mathbf{E}_n$, we have $\mathbf{S}_n$ is equal to $\frac{1}{n-1}\mathbf{X}\mathbf{E}_n\mathbf{X}^T$.

b) The result of PCA is $\mathbf{Q}(\mathbf{x}_i - \overline{\mathbf{x}})$. This is indeed equal to $\mathbf{Q}(\mathbf{x}_i - \frac{1}{n}\mathbf{X}\mathbf{1}_n)$. Constructing the matrix $\mathbf{X}$ as suggested, the projected points can be written as:

$$\mathbf{Q}(\mathbf{X} - \frac{1}{n}\mathbf{X}\mathbf{1}_n\mathbf{1}_n^T) = \mathbf{Q}\mathbf{X}\mathbf{E}_n.$$

c) Let the singular value decomposition of $\mathbf{X}\mathbf{E}_n$ be:

$$\mathbf{X}\mathbf{E}_n = \mathbf{U}_{p\times p}\mathbf{\Lambda}\mathbf{V}_{n\times p}{}^T.$$

It is known that:

$$\mathbf{S}_n = \frac{1}{n-1}\mathbf{U}\mathbf{\Lambda}^2\mathbf{U}^T,$$

and top k eigenvectors of $\mathbf{S}_n$ are given therefore by picking first k columns of $\mathbf{U}$, denoted by $\mathbf{U}_k$. In any case, we have:

$$\mathbf{U}_k^T\mathbf{X} = \begin{bmatrix} \mathbf{u}_1^T\mathbf{x}_1 & \dots & \mathbf{u}_1^T\mathbf{x}_n \\ \vdots & \ddots & \vdots \\ \mathbf{u}_k^T\mathbf{x}_1 & \dots & \mathbf{u}_k^T\mathbf{x}_n \end{bmatrix} = [\hat{\mathbf{x}}_1, \dots, \hat{\mathbf{x}}_n],$$

where $\hat{\mathbf{x}}_i$ is the projected point into the k dimensional subspace. From the previous point, the projected points are given by $\mathbf{U}_k^T\mathbf{X}\mathbf{E}_n$.

See that:

$$\mathbf{U}_k^T\mathbf{X}\mathbf{E}_n = \mathbf{U}_k^T\mathbf{U}\mathbf{\Lambda}\mathbf{V}^T.$$

But :

$$\mathbf{U}_k^T\mathbf{U} = \begin{bmatrix} \mathbf{u}_1^T\mathbf{u}_1 & \dots & \mathbf{u}_1^T\mathbf{u}_p \\ \vdots & \ddots & \vdots \\ \mathbf{u}_k^T\mathbf{u}_1 & \dots & \mathbf{u}_k^T\mathbf{u}_p \end{bmatrix} = [\mathbf{I}_k \quad \mathbf{0}_{k\times p-k}].$$

Using the fact that $\mathbf{\Lambda}_{ii}^2 = \lambda_i$, we have:

$$\mathbf{U}_k^T\mathbf{U}\mathbf{\Lambda} = [\mathbf{I}_k \quad \mathbf{0}_{k\times p-k}]\mathbf{\Lambda} = [\text{diag}(\sqrt{\lambda_1}, \sqrt{\lambda_2}, \dots, \sqrt{\lambda_k})_{k\times k} \quad \mathbf{0}_{k\times p-k}]$$

Now write $\mathbf{V} = [\mathbf{v}_1 \dots \mathbf{v}_p]$ where $\mathbf{v}_i \in \mathbb{R}^n$. We have:

$$\mathbf{U}_k^T\mathbf{U}\mathbf{\Lambda}\mathbf{V}^T = [\text{diag}(\sqrt{\lambda_1}, \sqrt{\lambda_2}, \dots, \sqrt{\lambda_k})_{k\times k} \quad \mathbf{0}_{k\times p-k}]\mathbf{V}^T = \begin{bmatrix} \sqrt{\lambda_1}\mathbf{v}_1^T \\ \vdots \\ \sqrt{\lambda_k}\mathbf{v}_k^T \end{bmatrix}$$

d) MDS starts by finding $-\frac{1}{2}\mathbf{E}_n\mathbf{D}^{(2)}\mathbf{E}_n$ which is $\mathbf{E}_n\mathbf{X}^T\mathbf{X}\mathbf{E}_n$ for Euclidean distance matrix. The spectral decomposition of $\mathbf{E}_n\mathbf{X}^T\mathbf{X}\mathbf{E}_n$ is then found by $\hat{\mathbf{V}}\,\text{diag}(\lambda_1, \dots, \lambda_n)\hat{\mathbf{V}}^T$ where $\hat{\mathbf{V}} = [\hat{\mathbf{v}}_1 \dots \hat{\mathbf{v}}_n]$ is the eigenvector matrix. Using SVD of $\mathbf{X}\mathbf{E}_n$ above we get:

$$\mathbf{E}_n\mathbf{X}^T\mathbf{X}\mathbf{E}_n = \mathbf{V}\mathbf{\Lambda}^2\mathbf{V}^T.$$

Therefore if $\mathbf{V} = [\mathbf{v}_1 \dots \mathbf{v}_p]$, then for $i = 1, \dots, p$ we have:

$$\hat{\mathbf{v}}_i = \mathbf{v}_i.$$

The solution to MDS is then $\mathbf{X}^{*T} = [\sqrt{\lambda_1}\mathbf{v}_1, \dots, \sqrt{\lambda_k}\mathbf{v}_k] \in \mathbb{R}^{n\times k}$. This means that:

$$\mathbf{U}_k^T\mathbf{U}\mathbf{\Lambda}\mathbf{V}^T = \mathbf{X}^*.$$

It shows that applying MDS on the distance matrix $\mathbf{D}(\mathbf{X})$ provides the same result as PCA.

Remark: There is another way of showing this equivalence. Note that $\mathbf{S}_n = \frac{1}{n-1}\mathbf{X}\mathbf{E}_n\mathbf{X}^T$ and let $\mathbf{U}\mathbf{\Lambda}\mathbf{U}^T$ be its spectral decomposition. Suppose that $(\lambda, \mathbf{u})$ is eigenvalue-eigenvector of $\mathbf{X}\mathbf{E}_n\mathbf{X}^T = (\mathbf{X}\mathbf{E}_n)(\mathbf{X}\mathbf{E}_n)^T$. Then:

$$(\mathbf{X}\mathbf{E}_n)^T(\mathbf{X}\mathbf{E}_n)(\mathbf{X}\mathbf{E}_n)^T\mathbf{u} = \lambda(\mathbf{X}\mathbf{E}_n)^T\mathbf{u}.$$

This means that $(\mathbf{X}\mathbf{E}_n)^T\mathbf{u} = \mathbf{E}_n\mathbf{X}^T\mathbf{u}$ is an eigenvector of $(\mathbf{X}\mathbf{E}_n)^T(\mathbf{X}\mathbf{E}_n) = \mathbf{E}_n\mathbf{X}^T\mathbf{X}\mathbf{E}_n$ and λ is its eigenvalue. So top k eigenvalues of $\mathbf{X}\mathbf{E}_n\mathbf{X}^T$ remains the same for $\mathbf{E}_n\mathbf{X}^T\mathbf{X}\mathbf{E}_n$. Therefore $\mathbf{E}_n\mathbf{X}^T\mathbf{u}_1, \dots \mathbf{E}_n\mathbf{X}^T\mathbf{u}_k$ are top k eigenvectors of $\mathbf{E}_n\mathbf{X}^T\mathbf{X}\mathbf{E}_n$. They are orthogonal but they do not have unit norm:

$$\mathbf{u}^T(\mathbf{X}\mathbf{E}_n)(\mathbf{X}\mathbf{E}_n)^T\mathbf{u} = \mathbf{u}^T\lambda\mathbf{u} = \lambda.$$

Therefore a normalization by $\frac{1}{\sqrt{\lambda}}$ is needed. So top k eigenvectors of $\mathbf{E}_n\mathbf{X}^T\mathbf{X}\mathbf{E}_n$ is given by $\frac{1}{\sqrt{\lambda_1}}\mathbf{E}_n\mathbf{X}^T\mathbf{u}_1, \dots, \frac{1}{\sqrt{\lambda_k}}\mathbf{E}_n\mathbf{X}^T\mathbf{u}_k$. Therefore $\mathbf{X}^*_{\text{MDS}}$ is given by:

$$\mathbf{X}^*_{\text{MDS}} = \begin{bmatrix} \sqrt{\lambda_1}\mathbf{v}_1^T \\ \vdots \\ \sqrt{\lambda_k}\mathbf{v}_k^T \end{bmatrix} = \begin{bmatrix} \sqrt{\lambda_1}(\frac{1}{\sqrt{\lambda_1}}\mathbf{E}_n\mathbf{X}^T\mathbf{u}_1)^T \\ \vdots \\ \sqrt{\lambda_k}(\frac{1}{\sqrt{\lambda_k}}\mathbf{E}_n\mathbf{X}^T\mathbf{u}_k)^T \end{bmatrix} = \begin{bmatrix} \mathbf{X}\mathbf{E}_n\mathbf{u}_1^T \\ \vdots \\ \mathbf{X}\mathbf{E}_n\mathbf{u}_k^T \end{bmatrix} = \mathbf{U}_k^T\mathbf{X}\mathbf{E}_n.$$

But we have seen above that $\mathbf{U}_k^T\mathbf{X}\mathbf{E}_n$ is X^*_{PCA} and therefore the desired result follows.

Solution of Problem 2

Consider four samples in $\mathbb{R}^3$ given as follows:

$$\mathbf{x}_1 = \begin{bmatrix} 1 \\ 2 \\ -3 \end{bmatrix}, \mathbf{x}_2 = \begin{bmatrix} 3 \\ -1 \\ -2 \end{bmatrix} \mathbf{x}_3 = \begin{bmatrix} -4 \\ 2 \\ 2 \end{bmatrix} \mathbf{x}_4 = \begin{bmatrix} -3 \\ -1 \\ 4 \end{bmatrix}.$$

MDS steps are as follows:

a) Find $\mathbf{E}_n\mathbf{X}^T\mathbf{X}\mathbf{E}_n$ where $\mathbf{X} = [\mathbf{x}_1 \dots \mathbf{x}_n]$.
In this step, $\mathbf{X}$ is obtained as:

$$\mathbf{X} = \begin{bmatrix} 1 & 3 & -4 & -3 \\ 2 & -1 & 2 & -1 \\ -3 & -2 & 2 & 4 \end{bmatrix}$$

We have:

$$\mathbf{E}_n\mathbf{X}^T\mathbf{X}\mathbf{E}_n = \begin{bmatrix} 15.875 & 11.625 & -9.125 & -18.375 \\ 11.625 & 21.375 & -18.375 & -14.625 \\ -9.125 & -18.375 & 15.875 & 11.625 \\ -18.375 & -14.625 & 11.625 & 21.375 \end{bmatrix}$$

b) Find spectral decomposition of $\mathbf{E}_n\mathbf{X}^T\mathbf{X}\mathbf{E}_n = \mathbf{V}\,\mathrm{diag}(\lambda_1, \dots, \lambda_n)\mathbf{V}^T$.
For this example eigenvalues and eigenvectors are given by:

$$\mathrm{diag}(\lambda_1, \dots, \lambda_n) = \begin{bmatrix} 61 \\ 13.5 \\ 0 \\ 0 \end{bmatrix}$$

$$\mathbf{V} = \begin{bmatrix} -0.45267873 & 0.5 & -0.65666815 & 0.25502096 \\ -0.54321448 & -0.5 & -0.31320188 & -0.63102251 \\ 0.45267873 & 0.5 & -0.28197767 & -0.71157191 \\ 0.54321448 & -0.5 & -0.62544394 & 0.17447155 \end{bmatrix}$$

c) $\mathbf{X}^*$ is given by $[\sqrt{\lambda_1}\mathbf{v}_1, \dots, \sqrt{\lambda_k}\mathbf{v}_k]^T$.

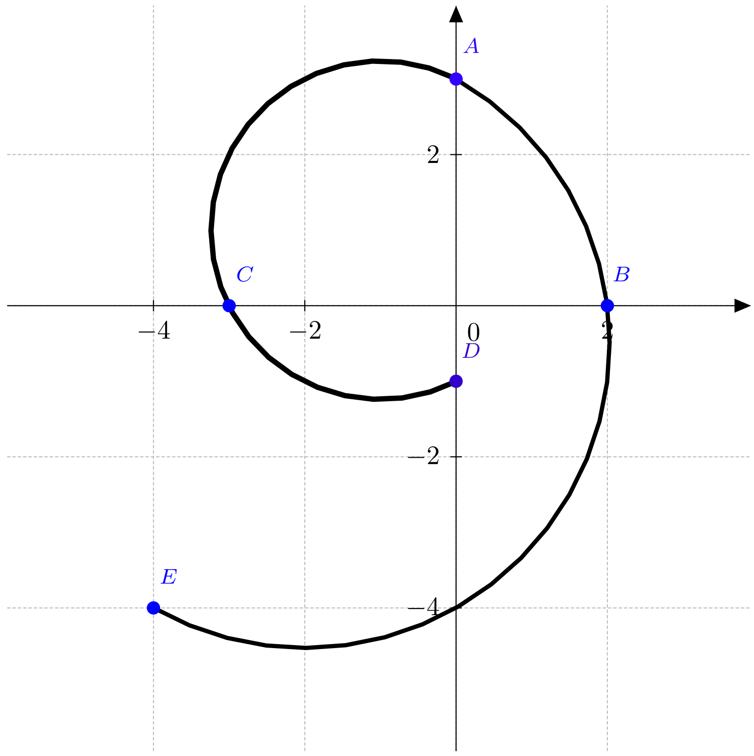
$$\mathbf{X}^{*T} = \begin{bmatrix} -3.53553391 & 1.83711731 \\ -4.24264069 & -1.83711731 \\ 3.53553391 & 1.83711731 \\ 4.24264069 & -1.83711731 \end{bmatrix}$$

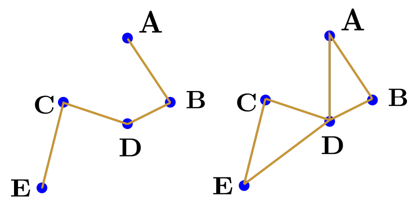
Checking with PCA process, similar output is found.

Solution of Problem 3

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

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

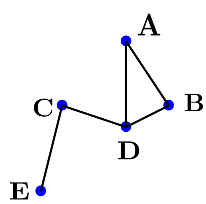




a) The following figure shows when 1NN and 2NN is used for graph construction. For 1NN graph $\delta(\mathbf{E}, \mathbf{D})$ is determined by a single path and is given by $\sqrt{10} + \sqrt{17}$. For 2NN graph, $\delta(\mathbf{E}, \mathbf{D})$ is the minimum of $\sqrt{32}$ and $\sqrt{10} + \sqrt{17}$, 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 $\epsilon > \sqrt{52}$.