# Theoretical Exercise 2

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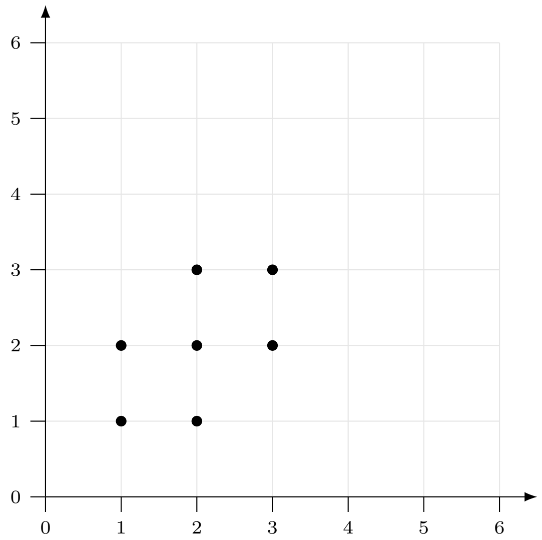
**This is the sample solution.**

## Exercise 1 Dimensionality Reduction

### (a) PCA

Compute a 1D embedding of the dataset below using PCA.



**Solution**

$X = \begin{pmatrix} 1 & 2 & 1 & 2 & 3 & 2 & 3 \\ 1 & 1 & 2 & 2 & 2 & 3 & 3 \end{pmatrix}, \mu = (2,2)^T$

$\hat{X} = X - \mu = \begin{pmatrix} -1 & 0 & -1 & 0 & 1 & 0 & 1 \\ -1 & -1 & 0 & 0 & 0 & 1 & 1 \end{pmatrix}$

$C = \frac{1}{n}\hat{X}\hat{X}^T = \frac{1}{8}\begin{pmatrix} 4 & 2 \\ 2 & 4 \end{pmatrix}$

compute Eigenvalues:

$|C - \lambda \cdot I| \stackrel{!}{=} 0$

$\Leftrightarrow \left| \frac{1}{8}\begin{pmatrix} 4 & 2 \\ 2 & 4 \end{pmatrix} - \begin{pmatrix} \lambda & 0 \\ 0 & \lambda \end{pmatrix} \right| = \left| \begin{pmatrix} 0.5-\lambda & 0.25 \\ 0.25 & 0.5-\lambda \end{pmatrix} \right| = (0.5-\lambda)^2 - \frac{1}{16} = 0$

$\Leftrightarrow (0.5 - \lambda) =^{+}_{-} \frac{1}{4}$

$\Leftrightarrow \lambda_1 = 0.75, \lambda_2 = 0.25$

compute Eigenvectors:

$C \cdot v_1 = \lambda_1 \cdot v_1$

$\Rightarrow (C - \lambda_1 I) \cdot v_1 = 0$

$\Rightarrow \begin{pmatrix} -0.25 & 0.25 \\ 0.25 & -0.25 \end{pmatrix} \cdot v_1 = 0 \Rightarrow v_1 = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}, \begin{pmatrix} 0.25 & 0.25 \\ 0.25 & 0.25 \end{pmatrix} \cdot v_2 = 0 \Rightarrow v_2 = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}$

use Eigenvector to largest Eigenvalue for projection:

$X_{proj} = v_1^T \cdot \hat{X} = \frac{1}{\sqrt{2}}\begin{pmatrix} -2 & -1 & -1 & 0 & 1 & 1 & 2 \end{pmatrix}$

## (b) MDS

What assumption does MDS make about the distance matrix? What can happen if that assumption does not hold?

**Solution**

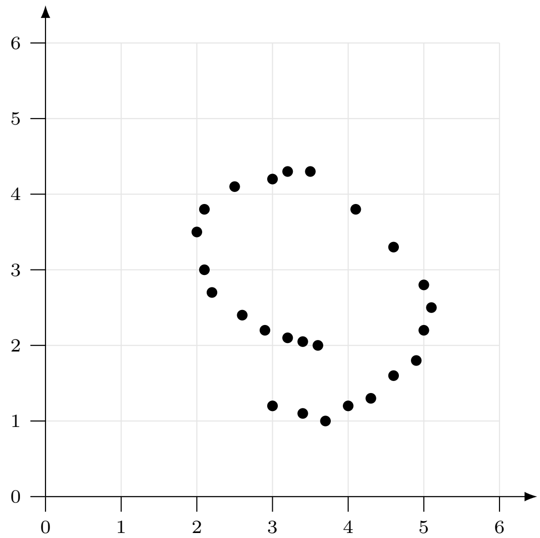
Repetition MDS:

$$\begin{aligned} d_{ij}^2 &= ||x_i - x_j||_2^2 = x_i^T x_i + x_j^T x_j - 2x_i^T x_j \\ B &= X^T X \\ B &= -\frac{1}{2} J^T D_2 J = V \Lambda V^T \\ X &= \Lambda^{\frac{1}{2}} V^T \\ X_p &= \Lambda_p^{\frac{1}{2}} V_p^T \end{aligned}$$

We assume that the distance matrix fullfills the triangle inequality $\Rightarrow$ there exists a Euclidean embedding $\Rightarrow$ B is positive semidefinite $\Rightarrow$ all Eigenvalues are positive.
If this were not the case we would not be able to tkae the square root for our decomposition.

## (c) IsoMap

How do we need to choose the neighbourhood size k in order for IsoMap to be able to preserve the structure (unrole the spiral), when embedding the dataset onto a 1D line?
What happens if we choose k smaller?
What happens if we chosse k bigger?




**Solution**

The graph needs to be connected, but there should not be any connection that does not preserve the structure.
Choose $k = 2$ or 3.
Smaller $k \Rightarrow$ disconnected components in the graph stucture $\Rightarrow$ Components are embedded arbitrarily far away.
Bigger $k \Rightarrow$ we have a connection between the tips of the spiral $\Rightarrow$ not possible to unroll any more.