MLT: Week-1

Standard PCA

A Aniruddha

Steps involved in PCA

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Step 5: Transform the original data by multiplying it with the selected eigenvectors(PC's) to obtain a lower-dimensional representation.

Observe the dataset

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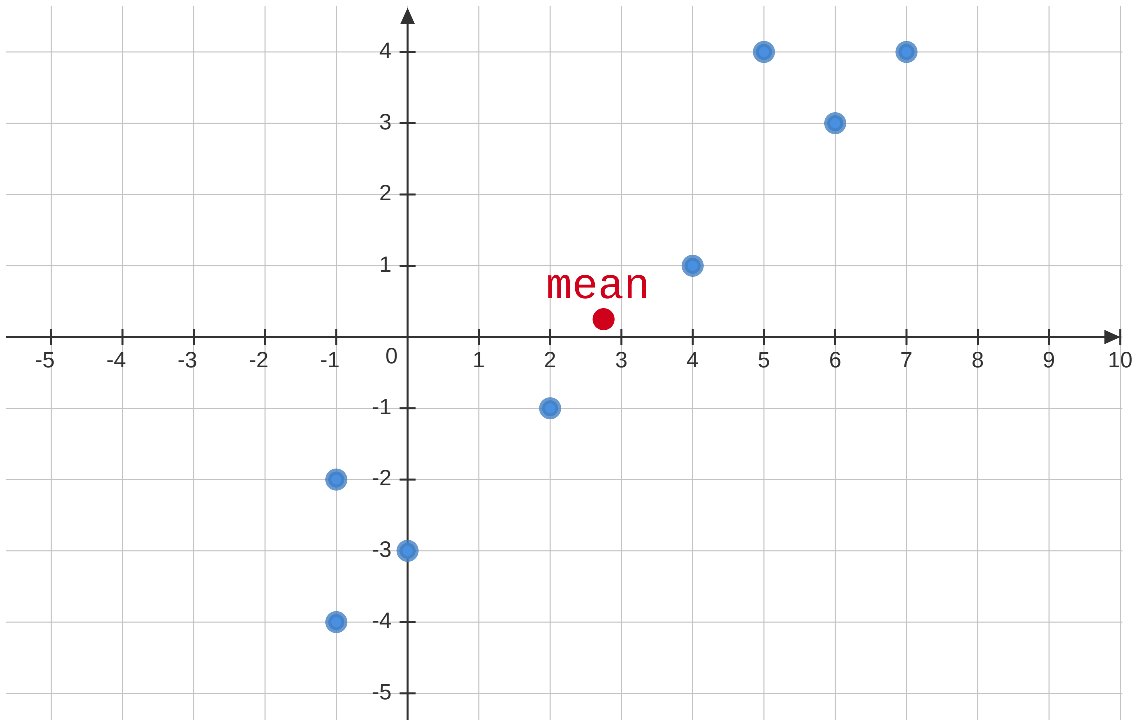

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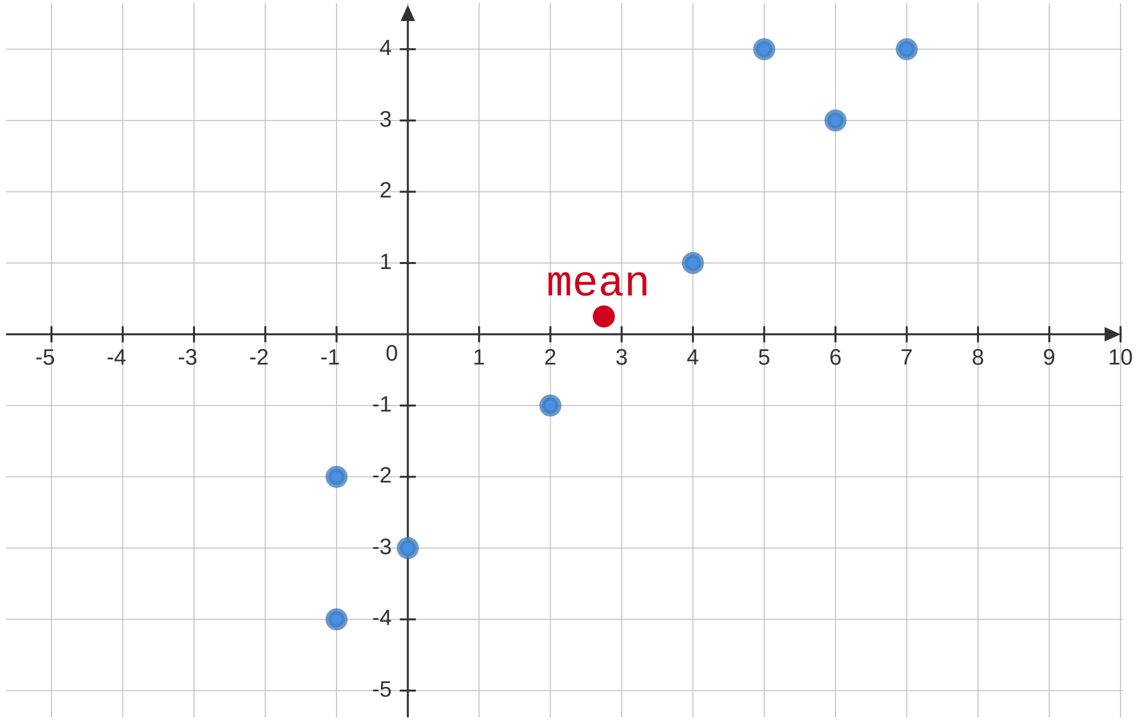

$$\mathbf{X} = \begin{bmatrix} 4 & 5 & 6 & 7 & 2 & -1 & 0 & -1 \\ 1 & 4 & 3 & 4 & -1 & -2 & -3 & -4 \end{bmatrix}$$

We can see that the dataset is not centered. Let us calculate the mean and center the dataset

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For the point $(4, 2)$, the value after updating will be:

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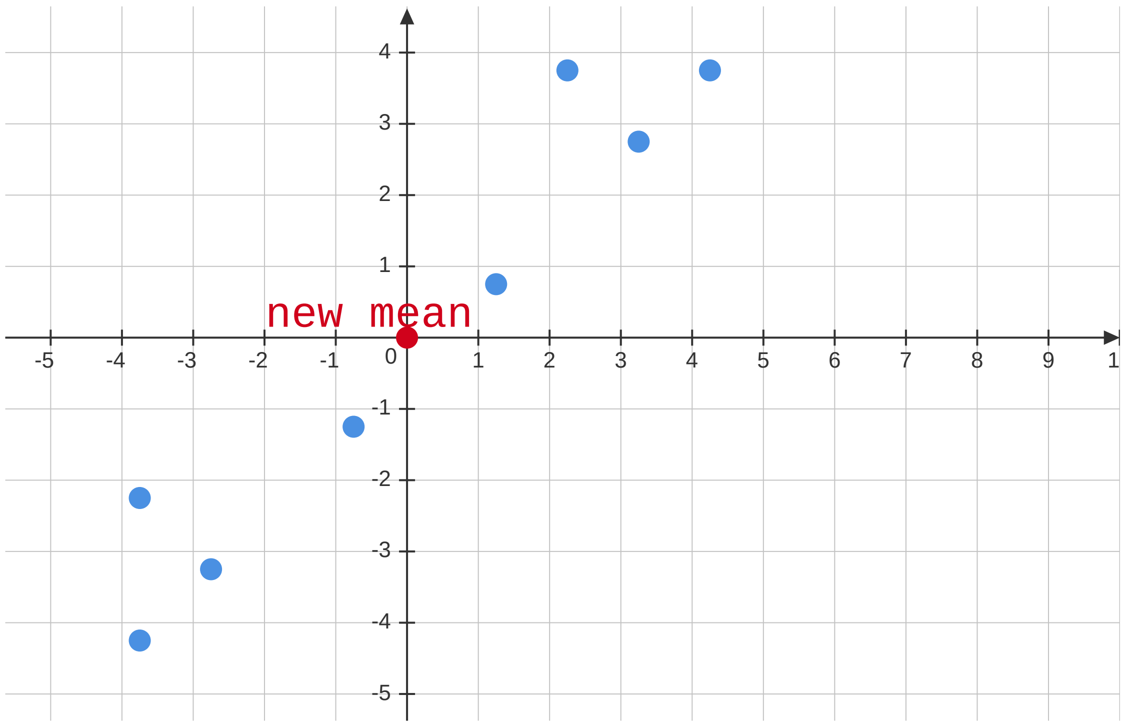

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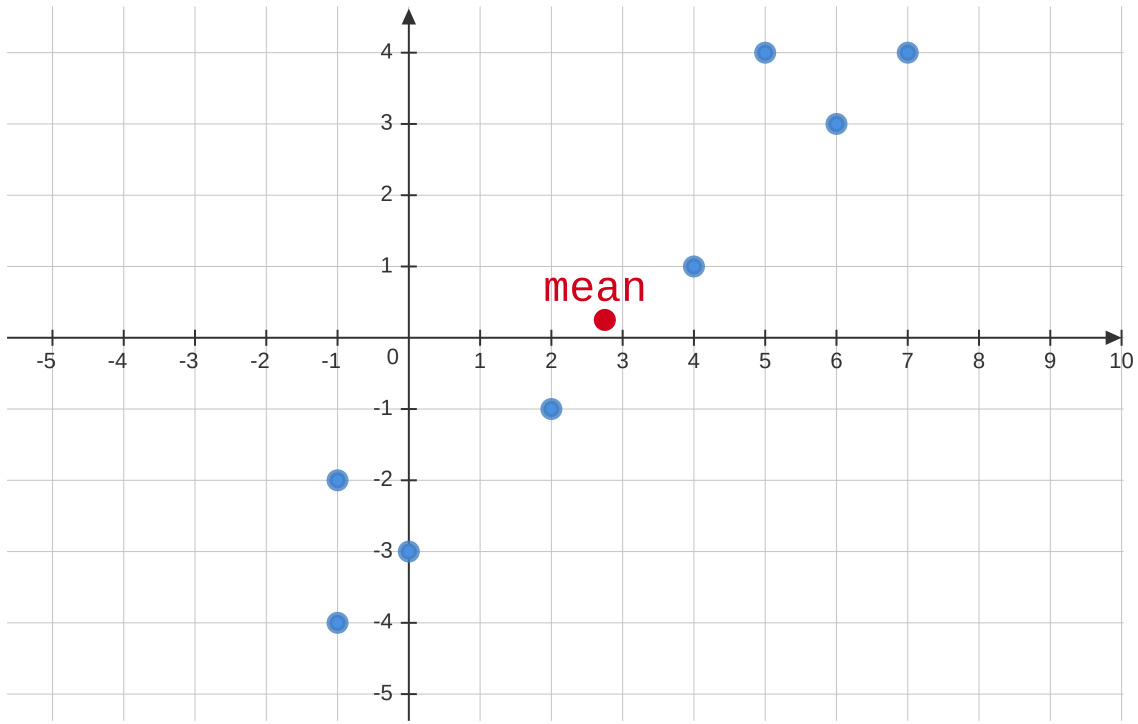
Dataset before centering



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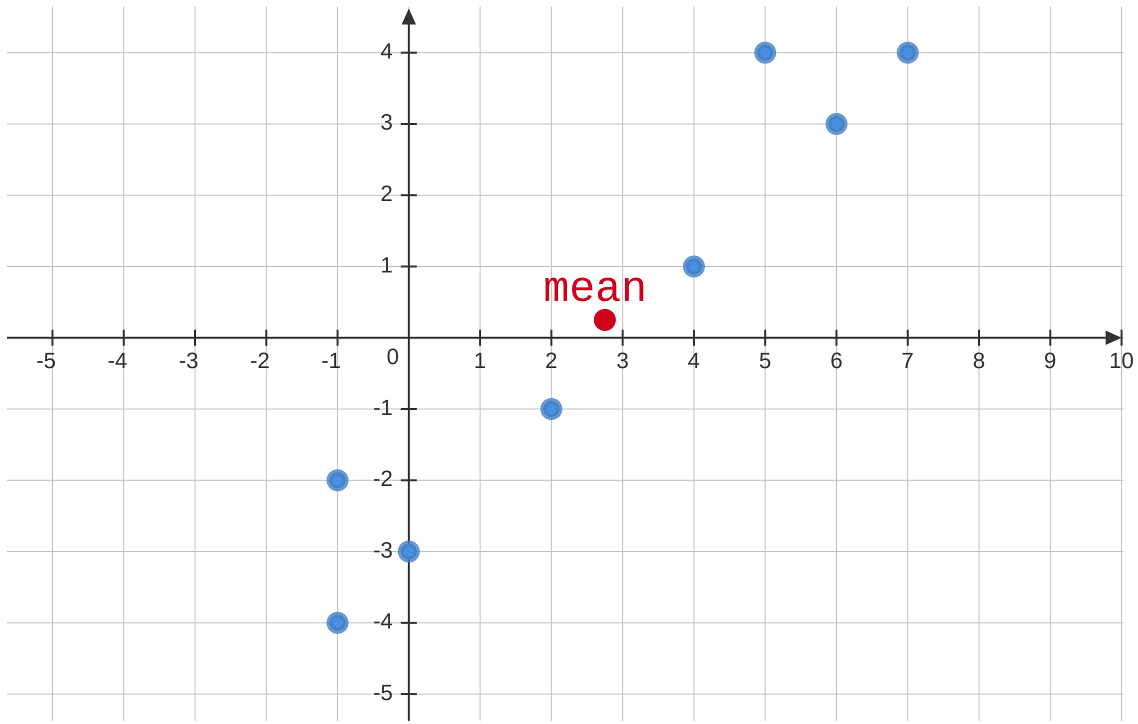

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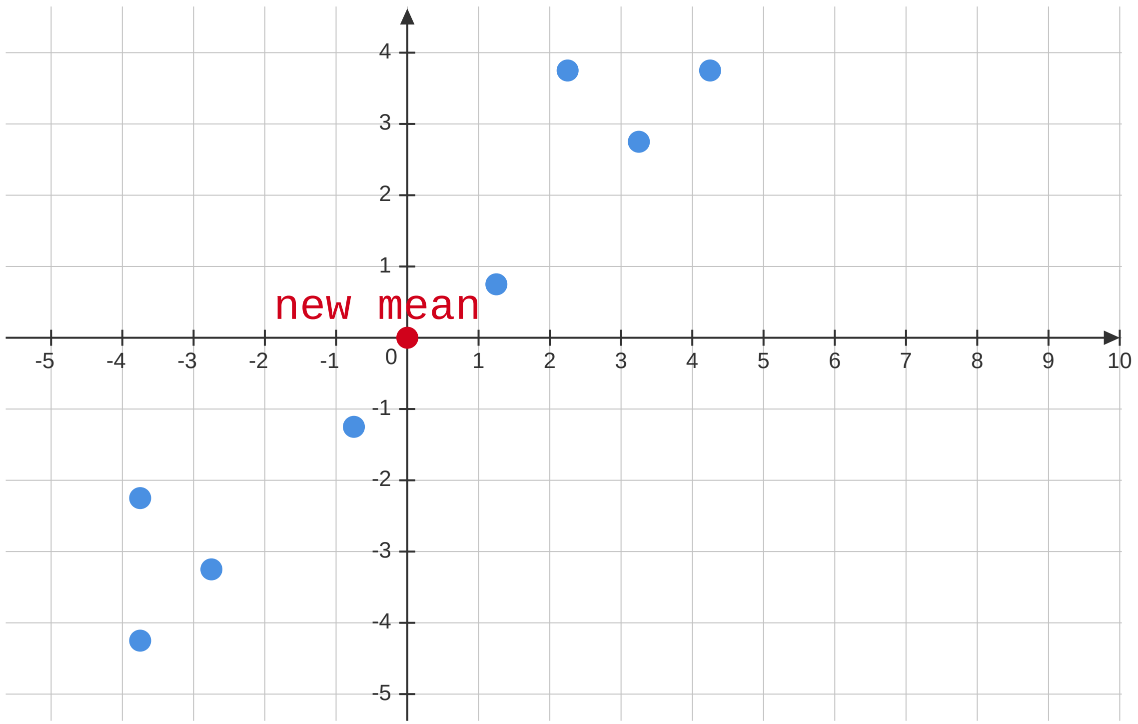

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The covariance matrix is given by $\mathbf{C} = \frac{1}{n}\sum_{i=1}^{n} x_i x_i^T = \frac{1}{n}\mathbf{X}\mathbf{X}^T$

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$$\mathbf{C} = \frac{1}{n}\mathbf{X}\mathbf{X}^T = \frac{1}{8}\begin{bmatrix} 71.5 & 68.5 \\ 68.5 & 71.5 \end{bmatrix}$$

$$= \begin{bmatrix} 8.9375 & 8.5625 \\ 8.5625 & 8.9375 \end{bmatrix}$$

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Now we calculate the eigenvalues and the corresponding eigenvectors of the covariance matrix

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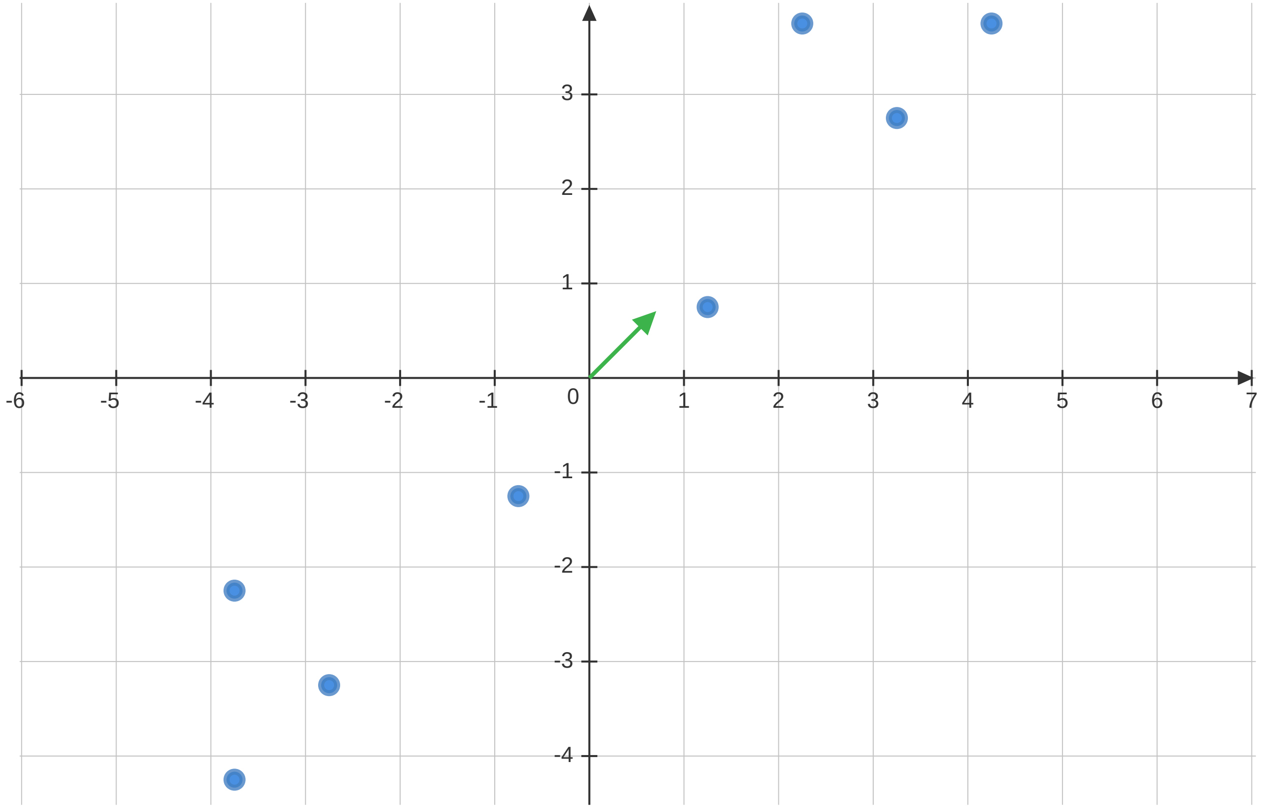
$$\lambda_1 = 17.5 \qquad \mathbf{w_1} = \begin{bmatrix} 0.707 \\ 0.707 \end{bmatrix}$$



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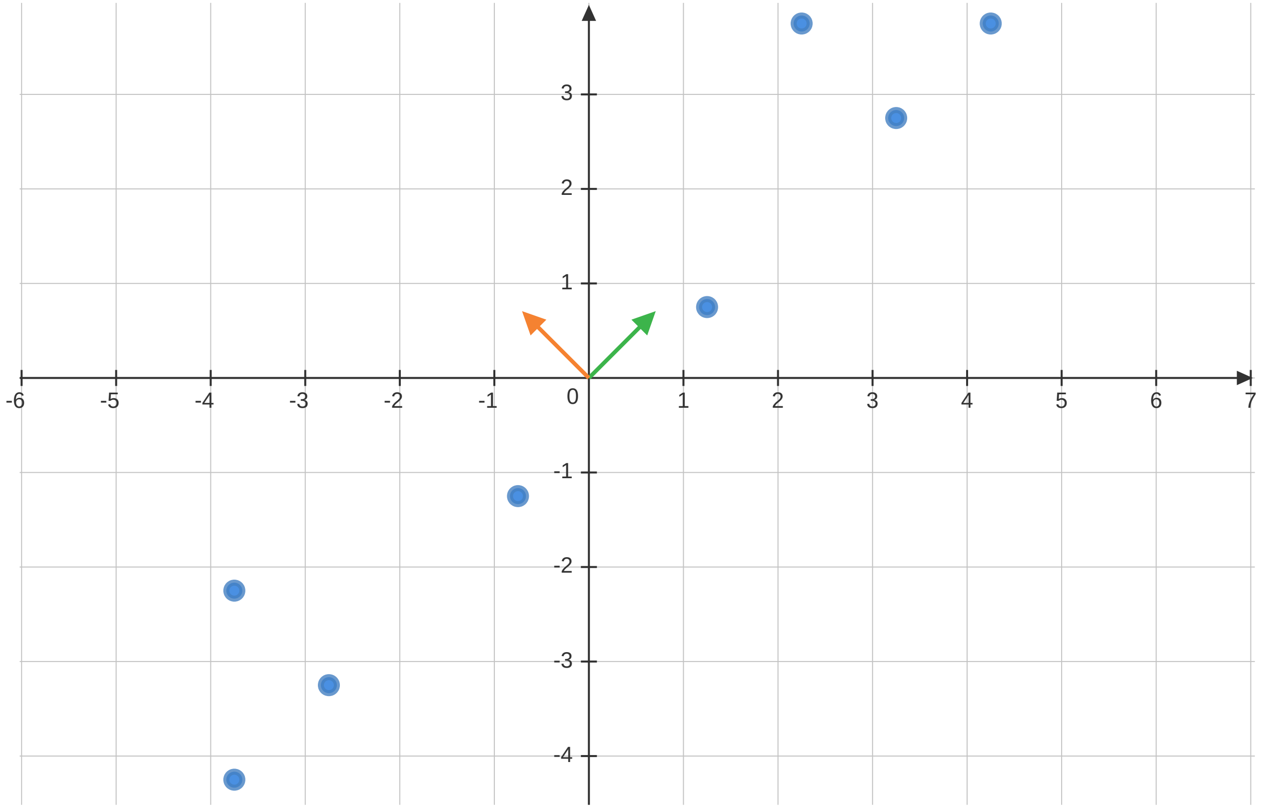
$$\lambda_1 = 17.5 \qquad \mathbf{w_1} = \begin{bmatrix} 0.707 \\ 0.707 \end{bmatrix}$$

$$\lambda_2 = 0.375 \qquad \mathbf{w_2} = \begin{bmatrix} -0.707 \\ 0.707 \end{bmatrix}$$



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How many principal components do we need to explain 95% of the variance in the dataset?

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The choice of k can be given by

$$\frac{\sum\limits_{i=1}^{k} \lambda_i}{\sum\limits_{i=1}^{d} \lambda_i} \geq 0.95$$

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The choice of k can be given by

$$\frac{\sum_{i=1}^{k} \lambda_i}{\sum_{i=1}^{d} \lambda_i} \geq 0.95$$

For k = 1, we have

$$\frac{\lambda_1}{\lambda_1 + \lambda_2} = \frac{17.5}{17.5 + 0.375}$$

$$= 0.979$$

Question - 2:

Represent the data using its two principal components and find the reconstruction error on each of these components

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$$\mathbf{w}_1 = \begin{bmatrix} 0.707 \\ 0.707 \end{bmatrix}$$

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To represent the datapoints along the kth principal component we simply need to multiply it with the the eigenvector corresponding to the kth-largest eigenvalue

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$$\left(\mathbf{X}^T_{\texttt{centered}} \cdot \mathbf{w}_1\right)^T = \begin{bmatrix} 1.414 & 4.242 & 4.242 & 5.656 & -1.414 & -4.242 & -4.242 & -5.656 \end{bmatrix}$$

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$$\left(\mathbf{X}^T_{\texttt{centered}} \cdot \mathbf{w}_2\right)^T = \begin{bmatrix} -0.353 & 1.060 & -0.353 & -0.353 & -0.353 & 1.060 & -0.353 & -0.353 \end{bmatrix}$$

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Represent the data using its two principal components and find the reconstruction error on each of these components

$$\text{Projection on first PC} = \mathbf{w}_1 \cdot \left(\mathbf{X}^T_{\texttt{centered}} \cdot \mathbf{w}_1\right)^T$$
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$$= \begin{bmatrix} 1 & 3 & 3 & 4 & -1 & -3 & -3 & -4 \\ 1 & 3 & 3 & 4 & -1 & -3 & -3 & -4 \end{bmatrix}$$

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$$\text{The matrix of reconstructed points is} = \begin{bmatrix} 1 & 3 & 3 & 4 & -1 & -3 & -3 & -4 \\ 1 & 3 & 3 & 4 & -1 & -3 & -3 & -4 \end{bmatrix}$$

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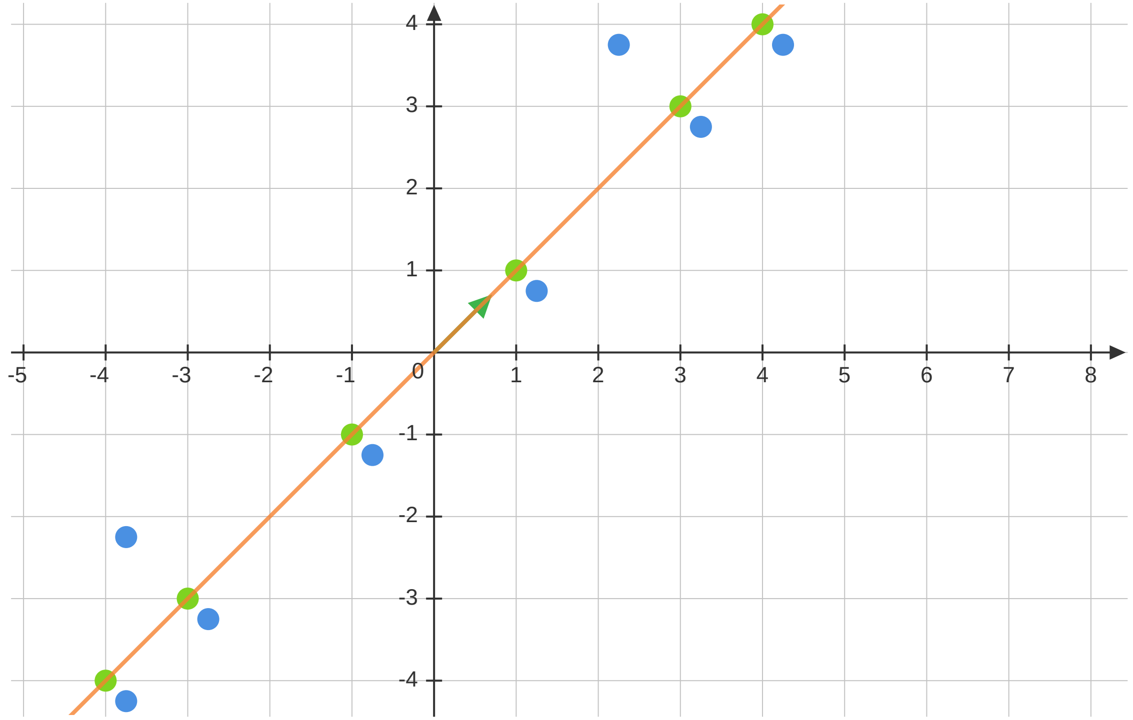

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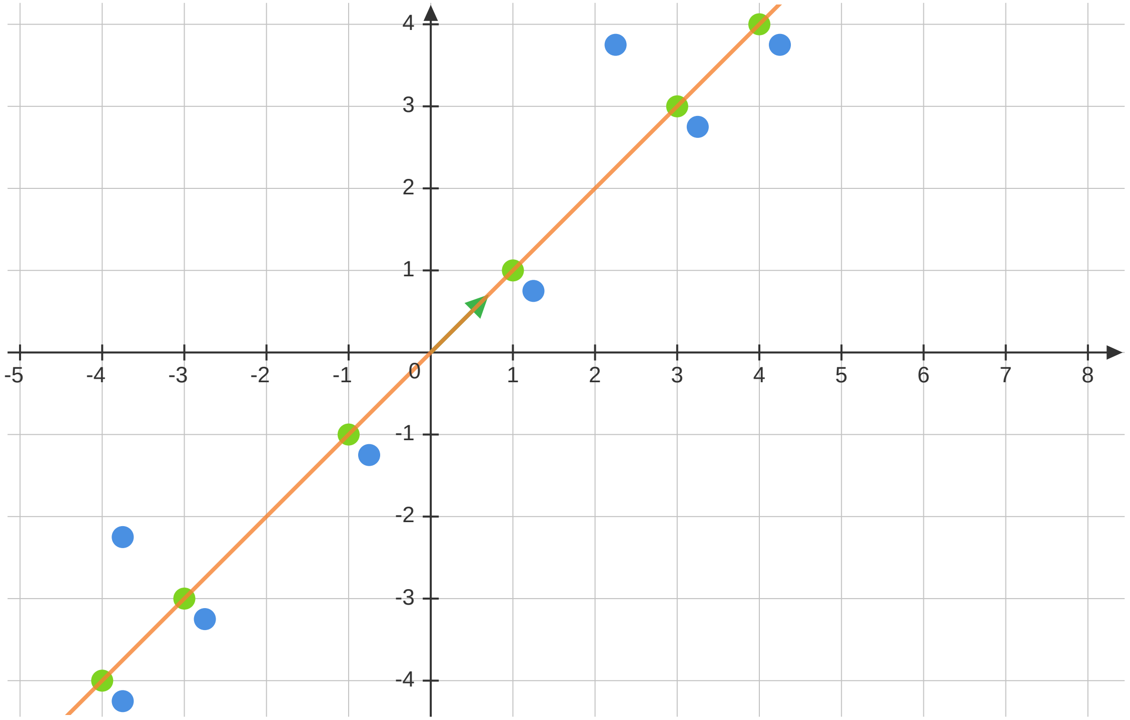

Comparison of the original dataset and the projected dataset

Question - 2:

Represent the data using its two principal components and find the reconstruction error on each of these components

$$\text{Projection on first PC} = \mathbf{w}_1 \cdot \left(\mathbf{X}_{\text{centered}}^T \cdot \mathbf{w}_1\right)^T$$
$$= \begin{bmatrix} 0.707 \\ 0.707 \end{bmatrix} \begin{bmatrix} 1.414 & 4.242 & 4.242 & 5.656 & -1.414 & -4.242 & -4.242 & -5.656 \end{bmatrix}$$
$$= \begin{bmatrix} 1 & 3 & 3 & 4 & -1 & -3 & -3 & -4 \\ 1 & 3 & 3 & 4 & -1 & -3 & -3 & -4 \end{bmatrix}$$

$$\text{Projection on second PC} = \mathbf{w}_2 \cdot \left(\mathbf{X}_{\text{centered}}^T \cdot \mathbf{w}_2\right)^T$$
$$= \begin{bmatrix} 0.707 \\ 0.707 \end{bmatrix} \begin{bmatrix} -0.353 & 1.060 & -0.353 & -0.353 & -0.353 & 1.060 & -0.353 & -0.353 \end{bmatrix}$$
$$= \begin{bmatrix} 0.25 & -0.75 & 0.25 & 0.25 & 0.25 & -0.75 & 0.25 & 0.25 \\ -0.25 & 0.75 & -0.25 & -0.25 & -0.25 & 0.75 & -0.25 & -0.25 \end{bmatrix}$$

Question - 2:

Represent the data using its two principal components and find the reconstruction error on each of these components

Adding the two projections, we get

$$= \begin{bmatrix} 1 & 3 & 3 & 4 & -1 & -3 & -3 & -4 \\ 1 & 3 & 3 & 4 & -1 & -3 & -3 & -4 \end{bmatrix} + \begin{bmatrix} 0.25 & -0.75 & 0.25 & 0.25 & 0.25 & -0.75 & 0.25 & 0.25 \\ -0.25 & 0.75 & -0.25 & -0.25 & -0.25 & 0.75 & -0.25 & -0.25 \end{bmatrix}$$

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$$= \begin{bmatrix} 1.25 & 2.25 & 3.25 & 4.25 & -0.75 & -3.75 & -2.75 & -3.75 \\ 0.75 & 3.75 & 2.75 & 3.75 & -1.25 & -2.25 & -3.25 & -4.25 \end{bmatrix}$$

As the points are in $\mathbb{R}^2$, we can get back the original centered dataset when we use both the Principal Components

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

The first point of $\mathbf{X}^T_{\text{centered}}$ is $\begin{bmatrix} 1.25 \\ 0.75 \end{bmatrix}$ and the same point when reconstructed using the first principal component is given by $\begin{bmatrix} 1 \\ 1 \end{bmatrix}$

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The first point of $\mathbf{X}^T_{\texttt{centered}}$ is $\begin{bmatrix} 1.25 \\ 0.75 \end{bmatrix}$ and the same point when reconstructed using the first principal component is given by $\begin{bmatrix} 1 \\ 1 \end{bmatrix}$

$$\text{The reconstruction error for this point is given by} = \texttt{length}^2(error)$$

$$= \| \mathbf{x}_1 - \left(\mathbf{x}_1^T \mathbf{w}_1\right)\mathbf{w}_1 \|^2$$

$$= (1.25 - 1)^2 + (0.75 - 1)^2$$

$$= 0.125$$

Question - 2:

Represent the data using its two principal components and find the reconstruction error on each of these components

The reconstruction error for all of the points in $\mathbf{X}_{\text{centered}}$ when reconstructed using the first principal component turns out to be,

$$\mathbf{e}_1 = \begin{bmatrix} 0.125 & 1.125 & 0.125 & 0.125 & 0.125 & 1.125 & 0.125 & 0.125 \end{bmatrix}$$

The MSE w.r.t to first PC will be $= 0.375$

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Represent the data using its two principal components and find the reconstruction error on each of these components

The reconstruction error for all of the points in $\mathbf{X}_{\text{centered}}$ when reconstructed using the first principal component turns out to be,

$$\mathbf{e}_1 = \begin{bmatrix} 0.125 & 1.125 & 0.125 & 0.125 & 0.125 & 1.125 & 0.125 & 0.125 \end{bmatrix}$$

$$\text{The MSE w.r.t to first PC will be} = 0.375$$

We can now take another unit-vector $\mathbf{w}_r = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$ and project $\mathbf{X}_{\text{centered}}$ on it. We will then find the reconstruction error and compare it with that of the first principal component

Question - 2:

Represent the data using its two principal components and find the reconstruction error on each of these components

$$\text{Projection on } \mathbf{w}_r = \mathbf{w}_r \cdot \left(\mathbf{X}^T_{\text{centered}} \cdot \ \mathbf{w}_r\right)^T$$

$$= \begin{bmatrix} 0 \\ 1 \end{bmatrix} \begin{bmatrix} 0.75 & 3.75 & 2.75 & 3.75 & -1.25 & -2.25 & -3.25 & -4.25 \end{bmatrix}$$

$$= \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0.75 & 3.75 & 2.75 & 3.75 & -1.25 & -2.25 & -3.25 & -4.25 \end{bmatrix}$$

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The reconstruction error for all of the points in $\mathbf{X}_{\text{centered}}$ when reconstructed using the vector $\mathbf{w}_r$ turns out to be,

$$\mathbf{e}_r \ = \begin{bmatrix} 1.5625 & 5.0625 & 10.5625 & 18.0625 & 0.5625 & 14.0625 & 7.5625 & 14.0625 \end{bmatrix}$$

The MSE w.r.t to $\mathbf{w}_r$ will be $= \ 8.9375$

Question - 2:

Represent the data using its two principal components and find the reconstruction error on each of these components

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$$= \begin{bmatrix} 0 \\ 1 \end{bmatrix} \begin{bmatrix} 0.75 & 3.75 & 2.75 & 3.75 & -1.25 & -2.25 & -3.25 & -4.25 \end{bmatrix}$$

$$= \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0.75 & 3.75 & 2.75 & 3.75 & -1.25 & -2.25 & -3.25 & -4.25 \end{bmatrix}$$

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The MSE w.r.t to $\mathbf{w}_r$ will be $= \ 8.9375$

We observe that the reconstruction error when the points are projected on a vector $\mathbf{w}_r$ is higher as compared to the error when projected on the first principal component

Question - 3:

You are given $\mathbf{w_1} = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ 1 \end{bmatrix}$ as the first principal component. Among the following, which of them could be the second principal component?

(a) $\frac{1}{\sqrt{2}}\begin{bmatrix} 0 \\ 1 \end{bmatrix}$ (b) $\frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ 0 \end{bmatrix}$ (c) $\frac{1}{\sqrt{2}}\begin{bmatrix} -1 \\ 1 \end{bmatrix}$ (d) $\frac{1}{\sqrt{2}}\begin{bmatrix} -1 \\ -1 \end{bmatrix}$

Question - 3:

You are given $\mathbf{w_1} = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ 1 \end{bmatrix}$ as the first principal component. Among the following, which of them could be the second principal component?

(a) $\frac{1}{\sqrt{2}}\begin{bmatrix} 0 \\ 1 \end{bmatrix}$ (b) $\frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ 0 \end{bmatrix}$ (c) $\frac{1}{\sqrt{2}}\begin{bmatrix} -1 \\ 1 \end{bmatrix}$ (d) $\frac{1}{\sqrt{2}}\begin{bmatrix} -1 \\ -1 \end{bmatrix}$

We know that the principal components will be orthogonal to each other and based on that option (c) can be the second principal component.

$$\frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ 1 \end{bmatrix} \cdot \frac{1}{\sqrt{2}}\begin{bmatrix} -1 \\ 1 \end{bmatrix} = -\frac{1}{2} + \frac{1}{2} = 0$$