Principal Components Analysis (PCA)

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- a technique for finding patterns in data of high dimension

Outline:

1. Eigenvectors and eigenvalues

2. PCA:

    a) Getting the data

    b) Centering the data

    c) Obtaining the covariance matrix

    d) Performing an eigenvalue decomposition of the covariance matrix

    e) Choosing components and forming a feature vector

    f) Deriving the new data set

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Eigenvectors & eigenvalues:

$$\begin{bmatrix} 2 & 3 \\ 2 & 1 \end{bmatrix}$$

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Eigenvectors & eigenvalues:

$$\begin{bmatrix} 2 & 3 \\ 2 & 1 \end{bmatrix} * \begin{bmatrix} 1 \\ 3 \end{bmatrix}$$

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Eigenvectors & eigenvalues:

$$\begin{bmatrix} 2 & 3 \\ 2 & 1 \end{bmatrix} * \begin{bmatrix} 1 \\ 3 \end{bmatrix} = \begin{bmatrix} 11 \\ 5 \end{bmatrix}$$

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transformation matrix

eigenvector
(this vector and all multiples of it)

eigenvalue

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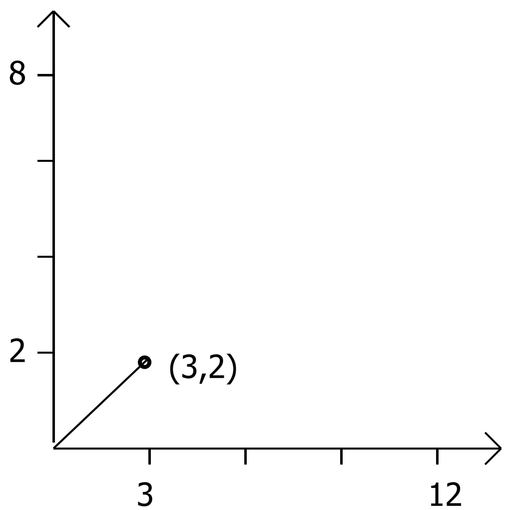

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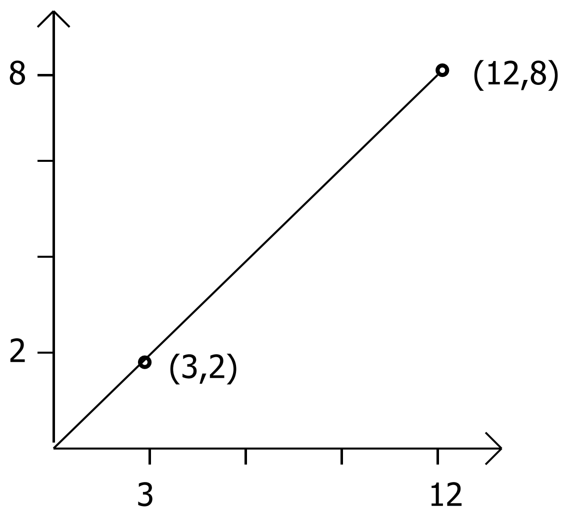

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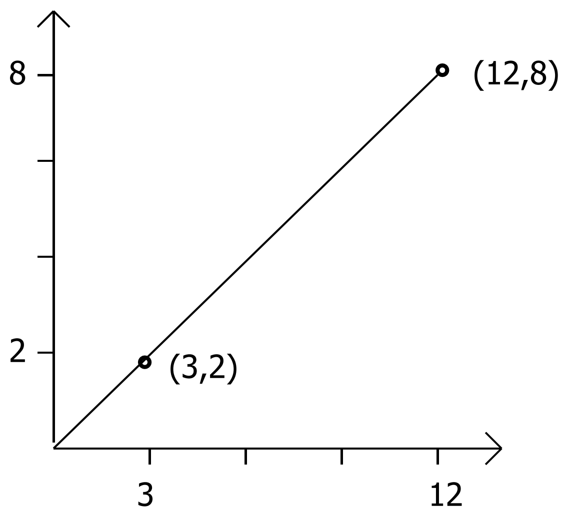

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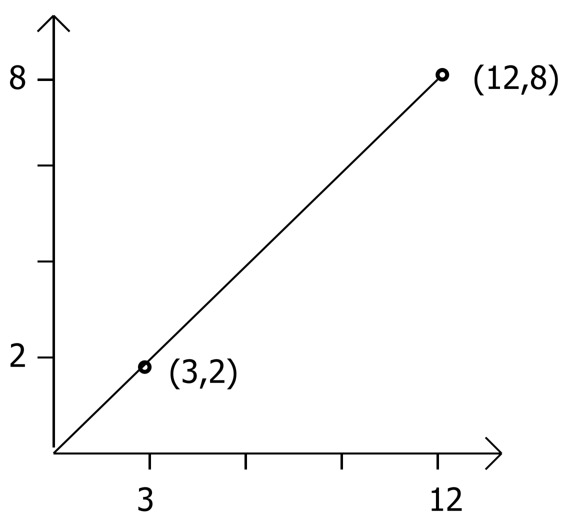

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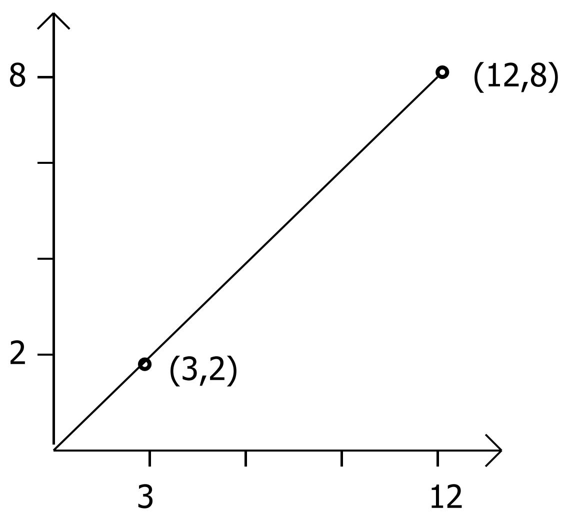
eigenvector (this vector and all multiples of it)



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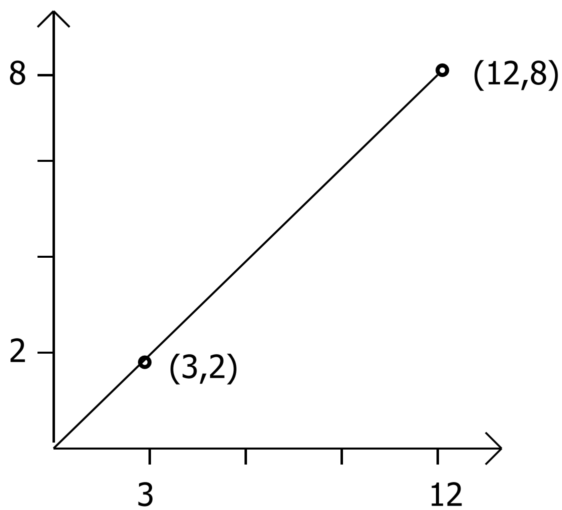

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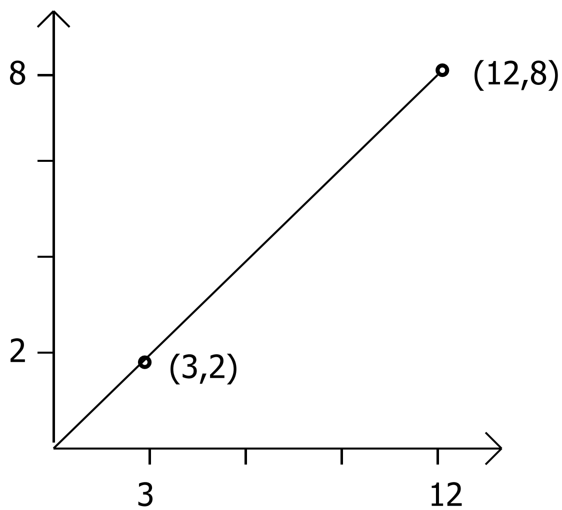

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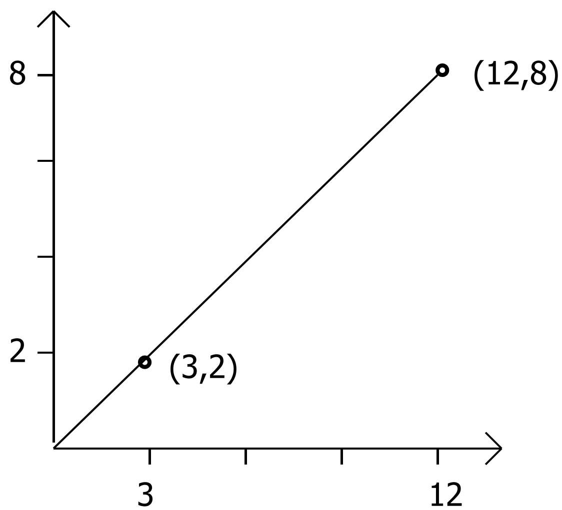

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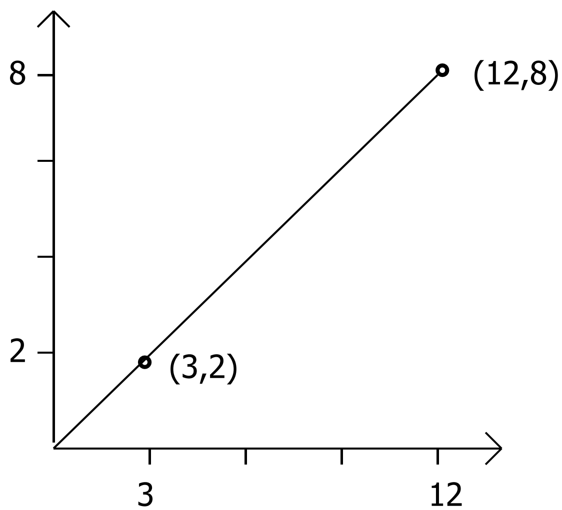

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$\longrightarrow$ not an integer multiple of the original vector

$$\begin{bmatrix}2 & 3\\ 2 & 1\end{bmatrix} * \begin{bmatrix}6\\ 4\end{bmatrix} = \begin{bmatrix} \\ \\ \end{bmatrix} = 4 *$$

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transformation matrix

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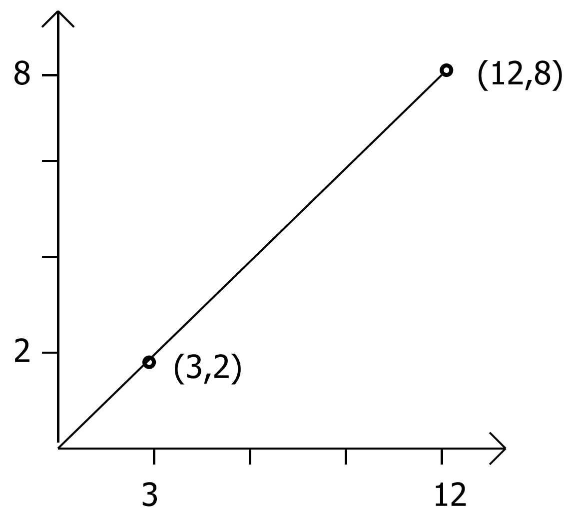

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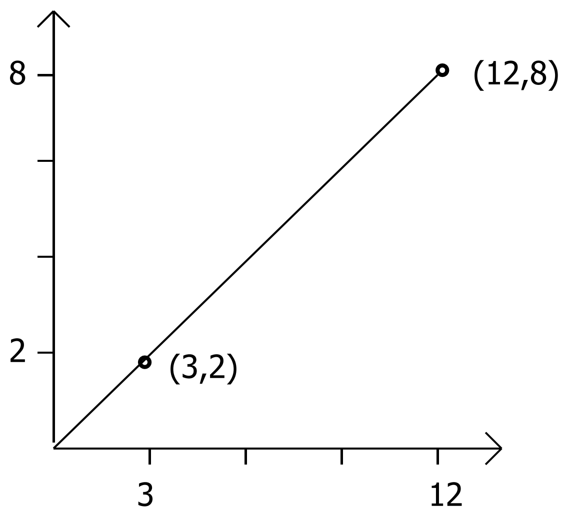

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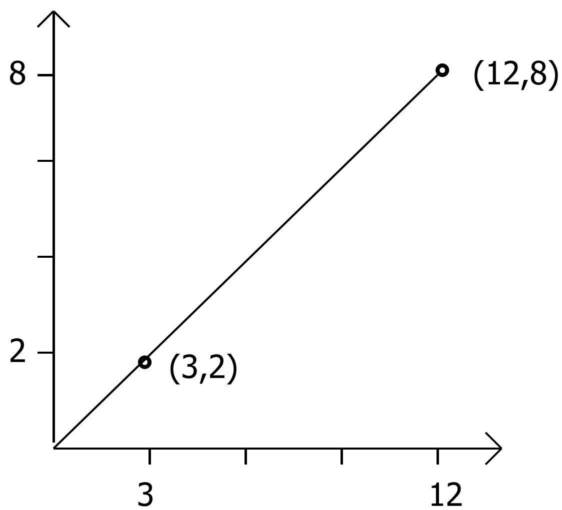

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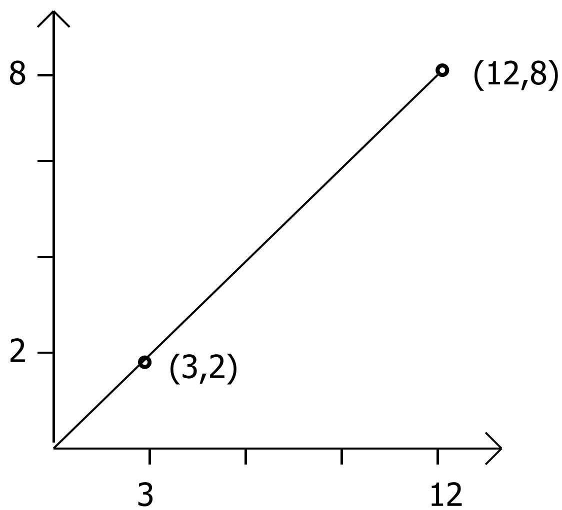

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- → thus, eigenvalues and eigenvectors come in pairs

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- a technique for identifying patterns in data and expressing the data in such a way as to highlight their similarities and differences

- once these patterns are found, the data can be compressed (i.e. the number of dimensions can be reduced) without much loss of information

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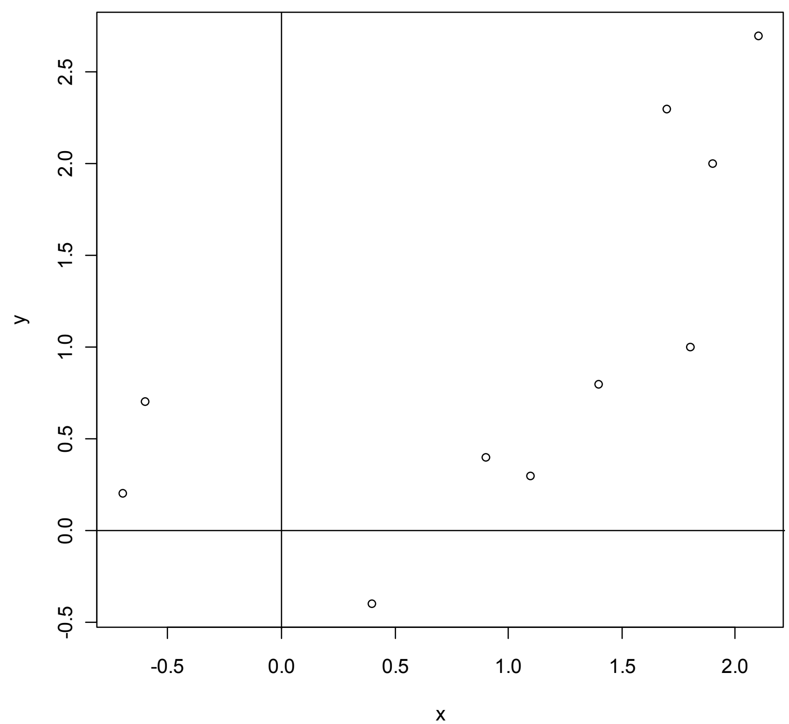
- example: data of 2 dimensions:

original data:

x	y
-0.7	0.2
2.1	2.7
1.7	2.3
1.4	0.8
1.9	2
1.8	1
0.4	-0.4
1.1	0.3
0.9	0.4
-0.6	0.7



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centered data:

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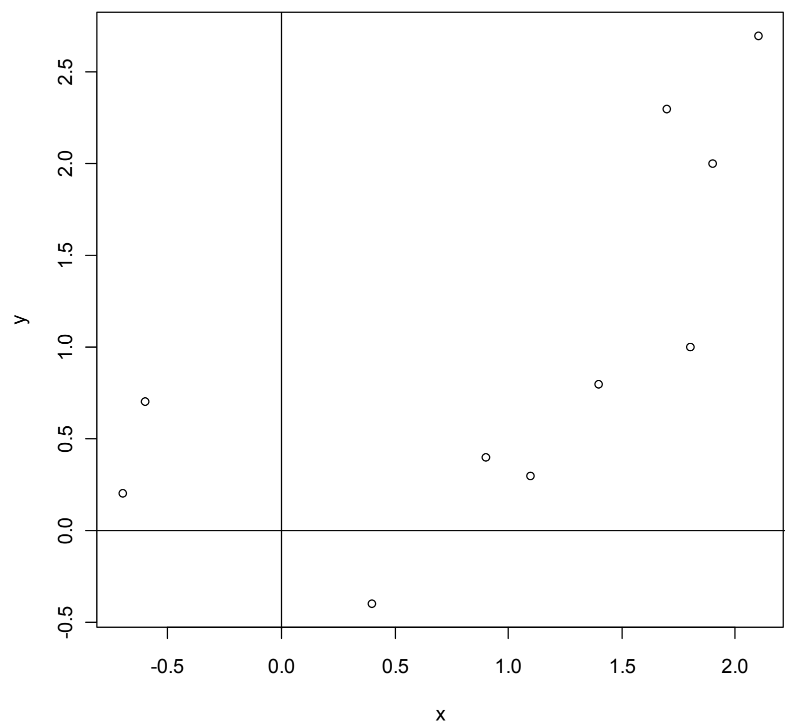

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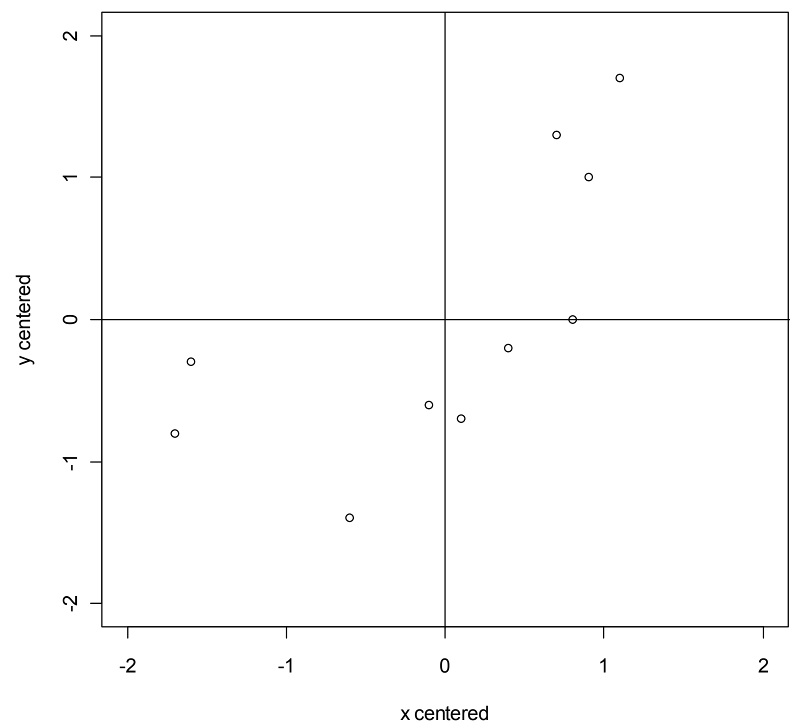

Covariance matrix:

$$\begin{array}{c c} & \begin{array}{cc} x & y \end{array} \\ \begin{array}{c} x \\ y \end{array} & \begin{bmatrix} 1.015556 & 0.696667 \\ 0.696667 & 1.017778 \end{bmatrix} \end{array}$$

Eigenvalues of the covariance matrix:

$$\begin{bmatrix} 1.7133342 \\ 0.3199991 \end{bmatrix}$$

Eigenvectors of the covariance matrix:

$$\begin{bmatrix} 0.706543 & -0.70767 \\ 0.70767 & 0.706543 \end{bmatrix}$$

* unit eigenvectors

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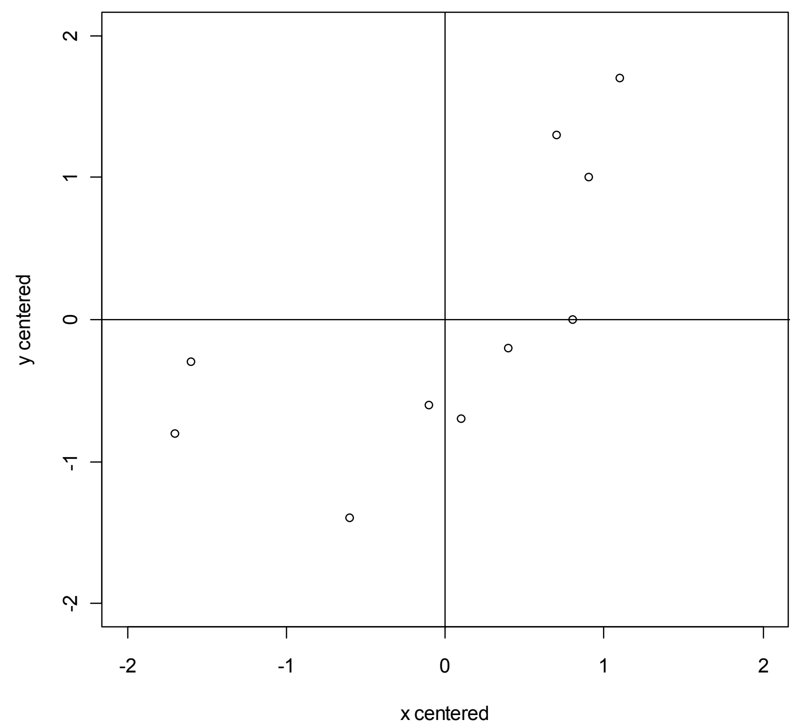

Covariance matrix:

$$\begin{array}{ccc} & x & y \\ x & \multicolumn{2}{c}{\multirow{2}{*}{}} \end{array}$$

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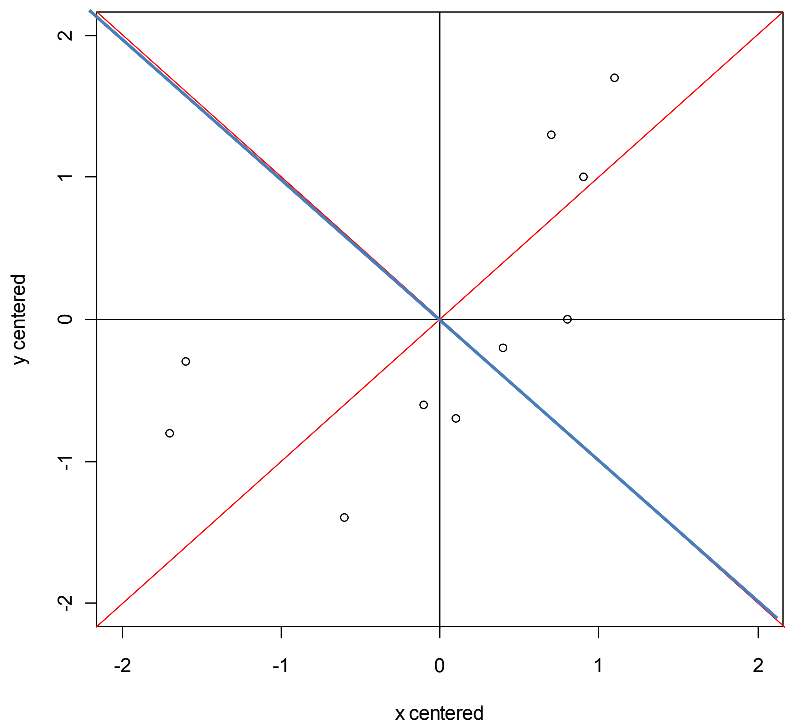


Compression and reduced dimensionality:

- the eigenvector associated with the highest eigenvalue is the principal component of the dataset; it captures the most significant relationship between the data dimensions

- ordering eigenvalues from highest to lowest gives the components in order of significance

- if we want, we can ignore the components of lesser significance – this results in a loss of information, but if the eigenvalues are small, the loss will not be great

- thus, in a dataset with n dimensions/variables, one may obtain the n eigenvectors & eigenvalues and decide to retain p of them → this results in a final dataset with only p dimensions

- feature vector – a vector containing only the eigenvectors representing the dimensions we want to keep – in our example data, 2 choices:

$$\begin{bmatrix} 0.706543 & -0.70767 \\ 0.70767 & 0.706543 \end{bmatrix} \quad \text{or} \quad \begin{bmatrix} 0.706543 \\ 0.70767 \end{bmatrix}$$

- the final dataset is obtained by multiplying the transpose of the feature vector (on the left) with the transposed original dataset

- this will give us the original data solely in terms of the vectors we chose

Our example:

a) retain both eigenvectors:

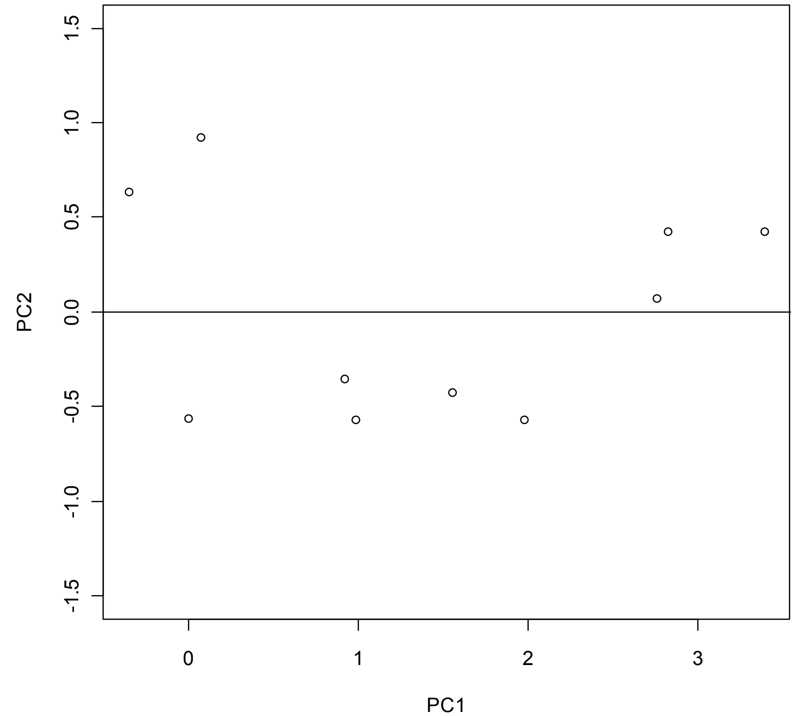
$$\begin{bmatrix} 0.706543 & 0.70767 \\ -0.70767 & 0.706543 \end{bmatrix} * \text{data}^{t} = \text{new data}$$

2x2   2x10   2x10

b) retain only the first eigenvector / principal component:

$$\begin{bmatrix} 0.706543 & 0.70767 \end{bmatrix} * \text{data}^{t} = \text{new data}$$

1x2   2x10   1x10



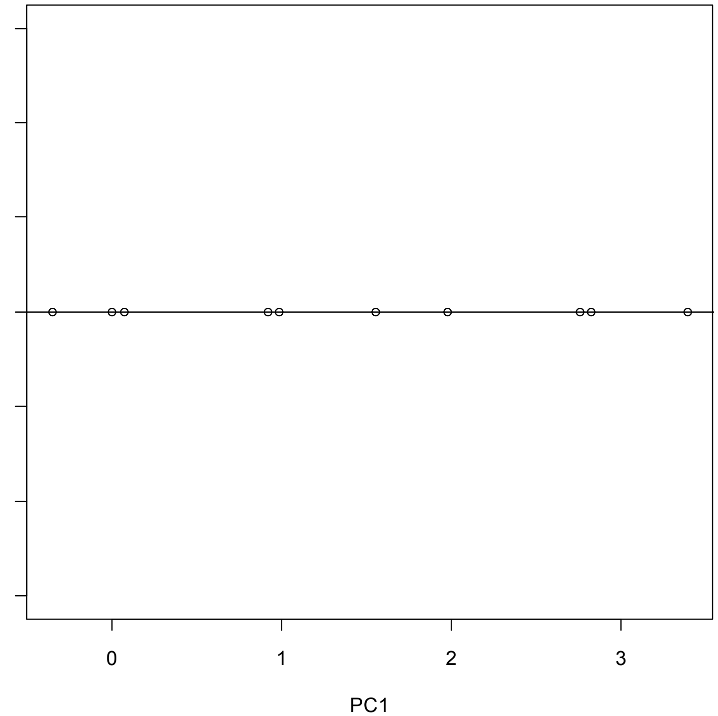
Original data, rotated so that the eigenvectors are the axes - no loss of information.

Our example:

a) retain both eigenvectors:

$$\begin{bmatrix} 0.706543 & 0.70767 \\ -0.70767 & 0.706543 \end{bmatrix} * \text{data}^{t} = \text{new data}$$

2x2   2x10   2x10



Original data, rotated so that the eigenvectors are the axes - no loss of information.

b) retain only the first eigenvector / principal component:

$$\begin{bmatrix} 0.706543 & 0.70767 \end{bmatrix} * \text{data}^{t} = \text{new data}$$

1x2   2x10   1x10

Only 1 dimension left – we threw away the other axis.

Thus: we transformed the data so that is expressed in terms of the patterns, where the patterns are the lines that most closely describe the relationships between the data.
Now, the values of the data points tell us exactly where (i.e., above/below) the trend lines the data point sits.

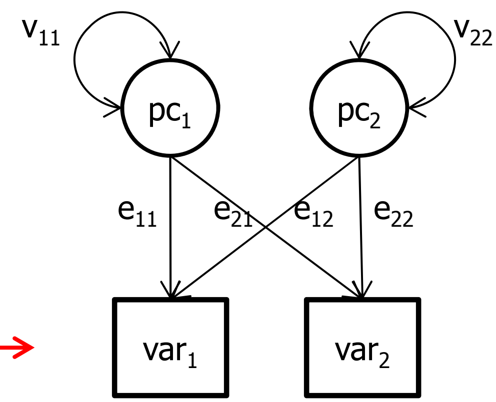
- similar to Cholesky decomposition as one can use both to fully decompose the original covariance matrix

- in addition, both produce uncorrelated factors

Eigenvalue decomposition:

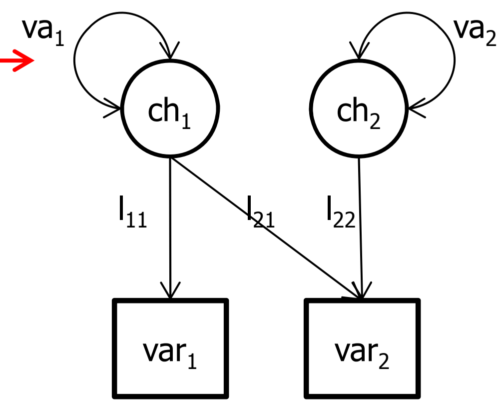
$$\begin{bmatrix} c_{11} & c_{21} \\ c_{21} & c_{22} \end{bmatrix} * \begin{bmatrix} e_{11} \\ e_{21} \end{bmatrix} = v1 * \begin{bmatrix} e_{11} \\ e_{21} \end{bmatrix}$$

$$\begin{bmatrix} c_{11} & c_{21} \\ c_{21} & c_{22} \end{bmatrix} = \begin{bmatrix} e_{11} & e_{12} \\ e_{21} & e_{22} \end{bmatrix} \begin{bmatrix} v_{11} & \\ & v_{22} \end{bmatrix} \begin{bmatrix} e_{11} & e_{12} \\ e_{21} & e_{22} \end{bmatrix}^{-1}$$



Cholesky decomposition:

$$\begin{bmatrix} c_{11} & c_{21} \\ c_{21} & c_{22} \end{bmatrix} = \begin{bmatrix} l_{11} & \\ l_{21} & l_{22} \end{bmatrix} \begin{bmatrix} va_{11} & \\ & va_{22} \end{bmatrix} \begin{bmatrix} l_{11} & l_{21} \\ & l_{22} \end{bmatrix}$$



Eigenvalue: decomposition

$C = E\ V\ E^{-1}$

Cholesky decomposition:

$C = \Lambda\ \Psi\ \Lambda^t$

Thank you for your attention.