



A tutorial on principal component analysis

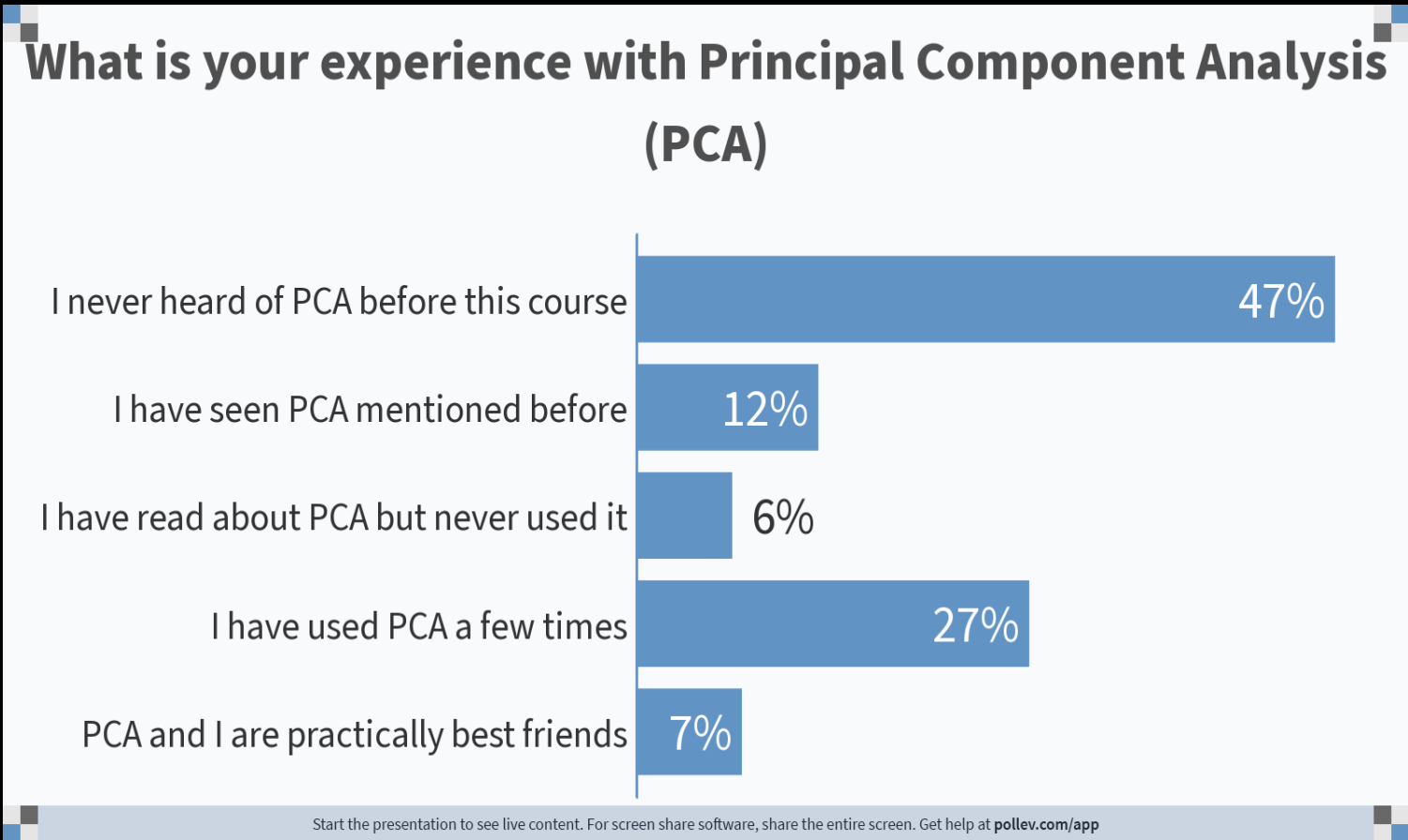
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DTU Compute

Based on

Jonathan Shlens: A tutorial on Principal Component Analysis (version 3.02
– April 7, 2014)

<http://compute.dtu.dk/courses/02502>





Principal Component Analysis (PCA) learning objectives

- Describe the concept of principal component analysis
- Explain why principal component analysis can be beneficial when there is high data redundancy
- Arrange a set of multivariate measurements into a matrix that is suitable for PCA analysis
- Compute the covariance of two sets of measurements
- Compute the covariance matrix from a set of multivariate measurements
- Compute the principal components of a data set using Eigenvector decomposition
- Describe how much of the total variation in the data set that is explained by each principal component

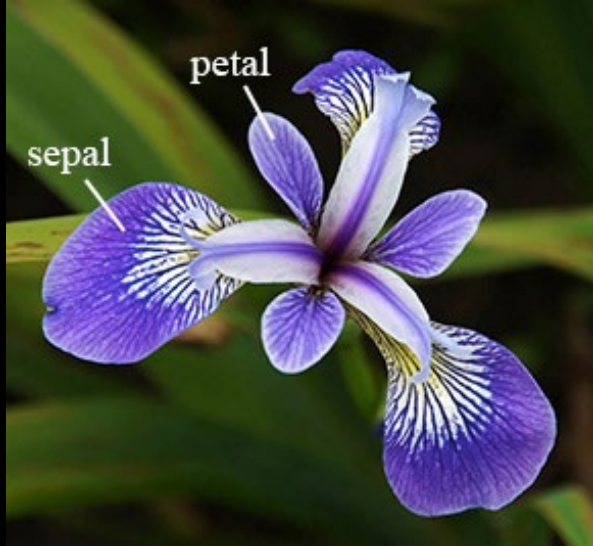


Iris data

The **Iris flower data** set or Fisher's Iris data set is a data set introduced by Ronald Fisher in his 1936 paper *The use of multiple measurements in taxonomic problems*



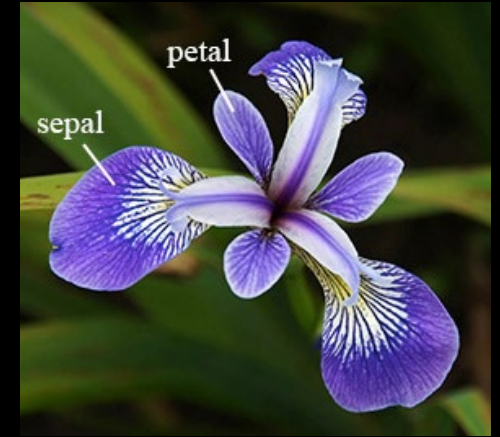
Iris data



- 3 Iris types
 - 50 flowers of each type
- For each flower
 - Sepal length
 - Sepal width
 - Petal length
 - Petal width
- We use one type as example
 - 50 measured flowers

Iris Data Matrix

- One column is one flower
- One row is all measurements of one type



$$\mathbf{X} = \begin{bmatrix}
 \begin{matrix} \text{Sepal length}_1 & \dots & \text{Sepal length}_{50} \\
 \text{Sepal width}_1 & \dots & \text{Sepal width}_{50} \\
 \text{Petal length}_1 & \dots & \text{Petal length}_{50} \\
 \text{Petal width}_1 & \dots & \text{Petal width}_{50} \end{matrix}
 \end{bmatrix}$$

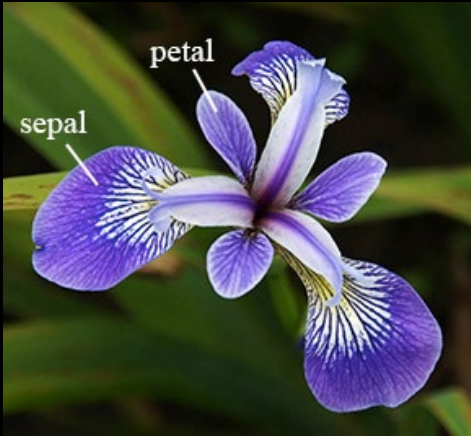


1



50

What can we use these data for?



- The measurements can be used to:
 - Recognize a species of flowers
 - Classify flowers into groups
 - Describe the characteristics of the flower
 - Quantify growth rates
 - ...

- Do we need all the measurements?
 - Can we *boil down* or *combine* some measurements?

- Are some measurements *redundant*?

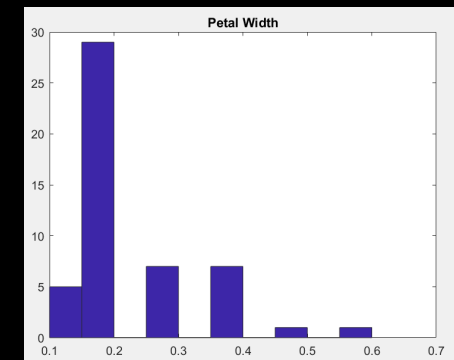
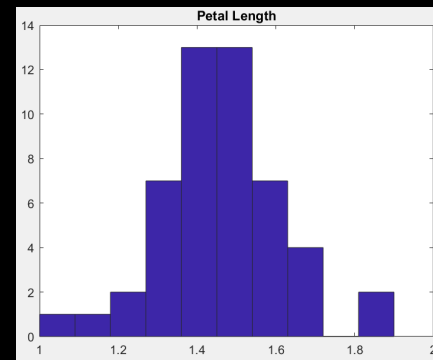
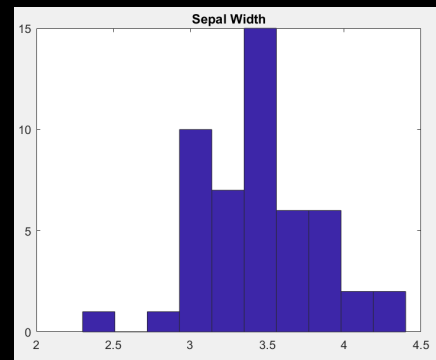
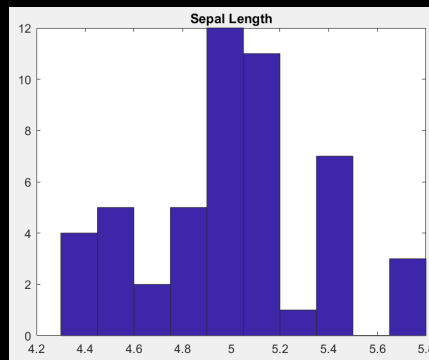
Variance

$$\sigma_{SL}^2 = 0.1242$$

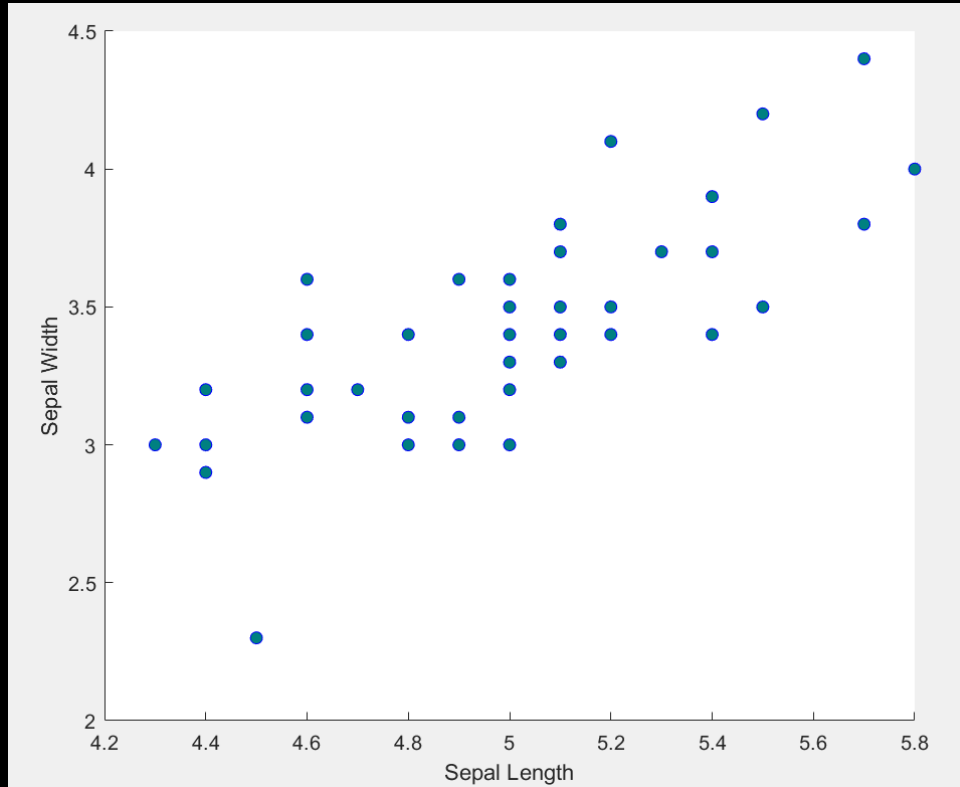
$$\sigma_{SW}^2 = 0.1437$$

$$\sigma_{PL}^2 = 0.0302$$

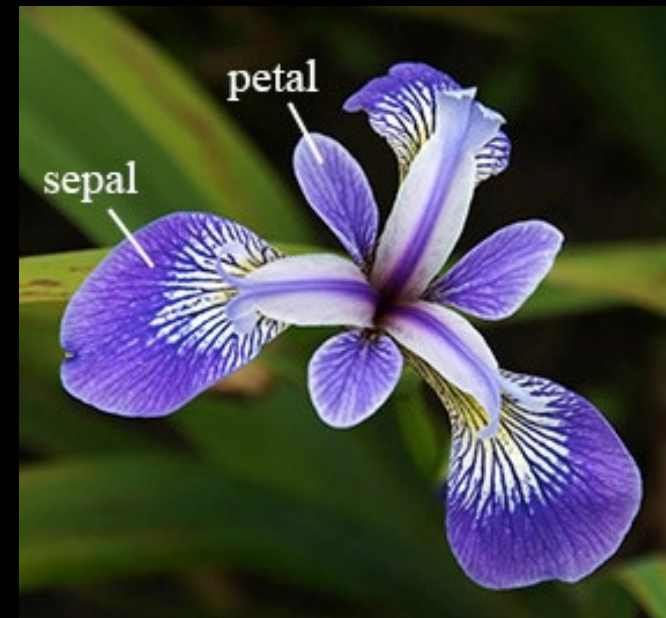
$$\sigma_{PW}^2 = 0.0111$$



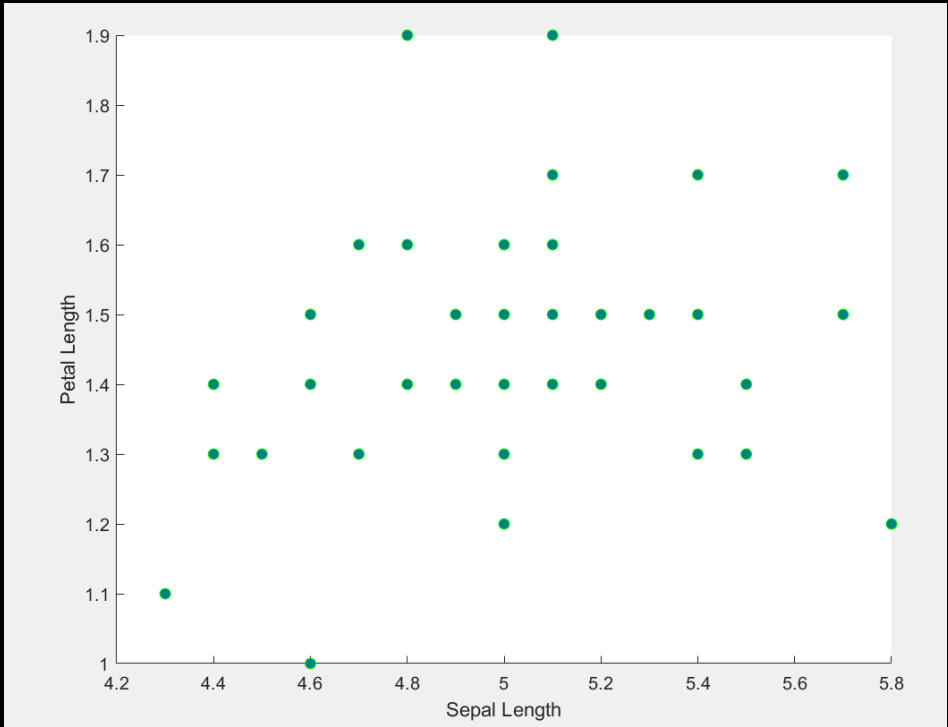
High Redundancy



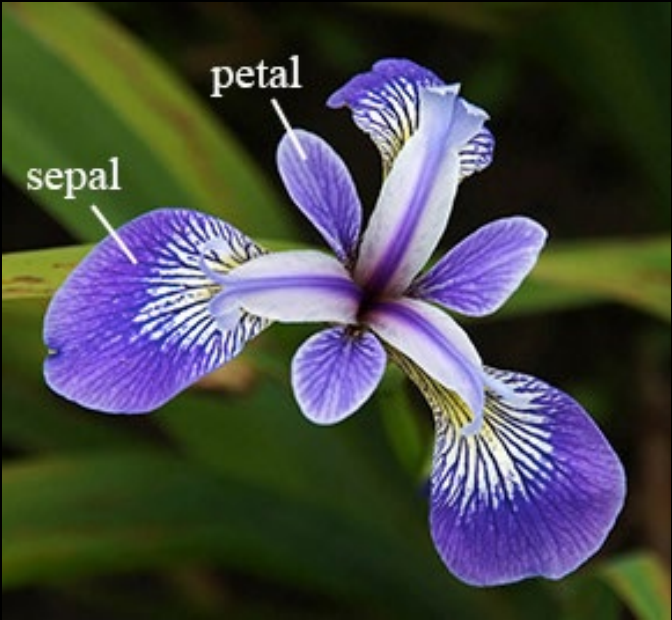
Observation: We can explain **quite a lot** of the sepal width if we know the sepal lengths



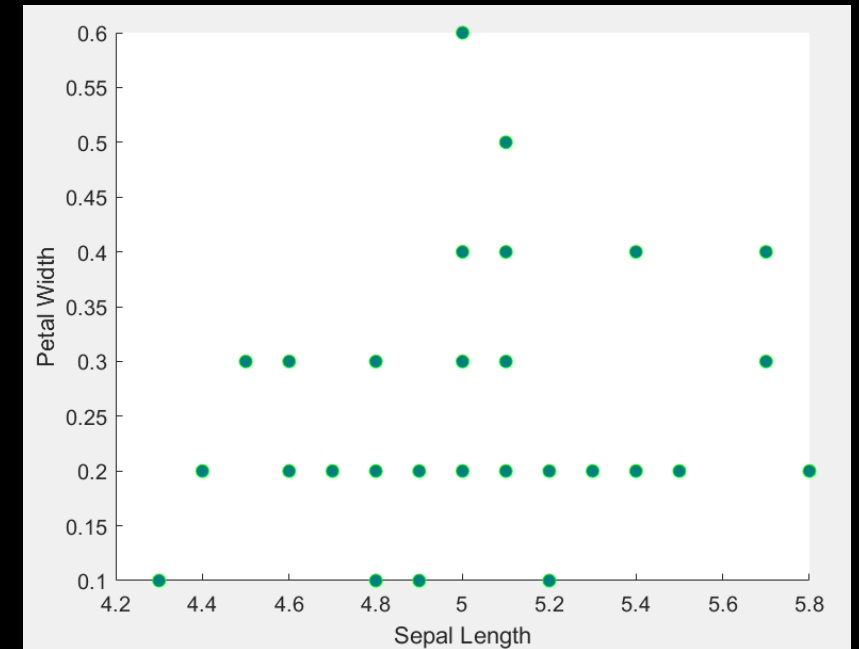
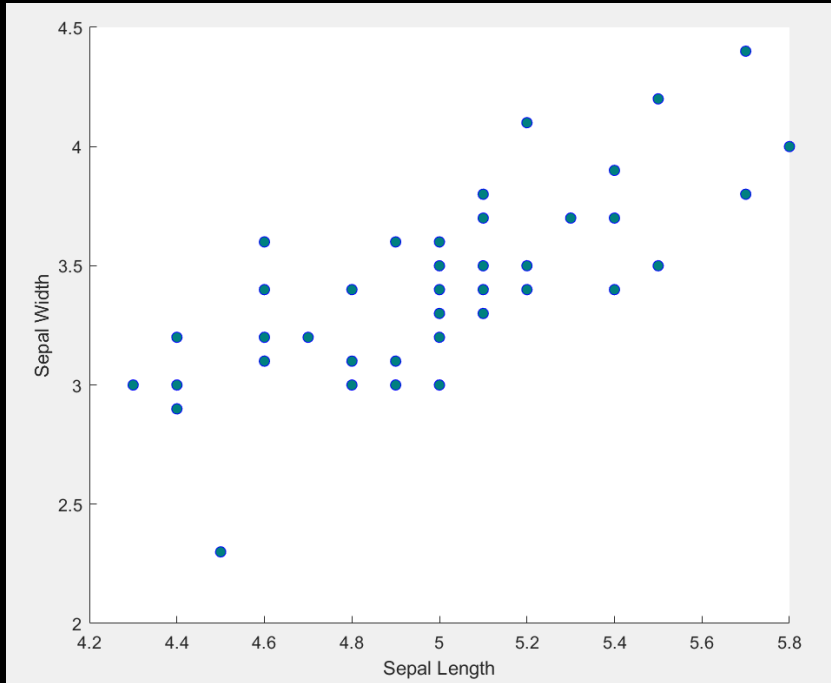
Low Redundancy



Observation: We can **NOT** explain the petal length if we know the sepal lengths

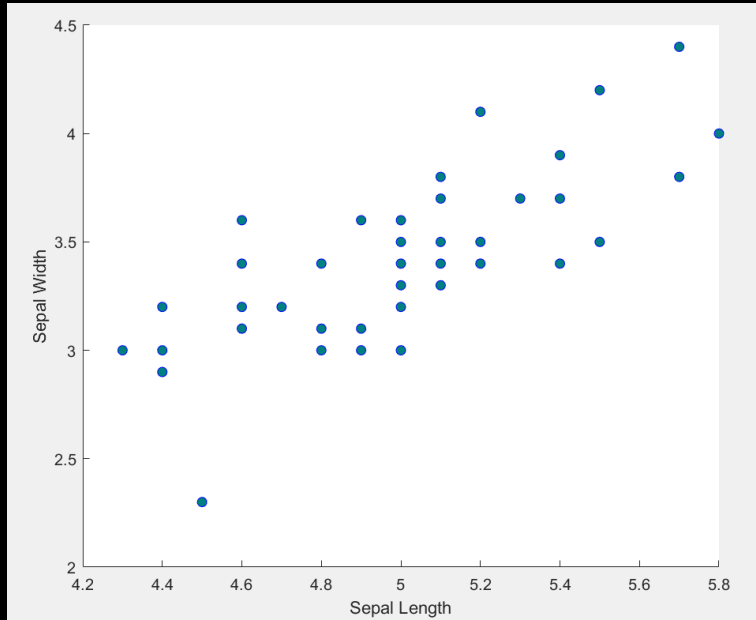


Covariance



Covariance measures the *relationship* between measurements

High Covariance



Sepal length and sepal width

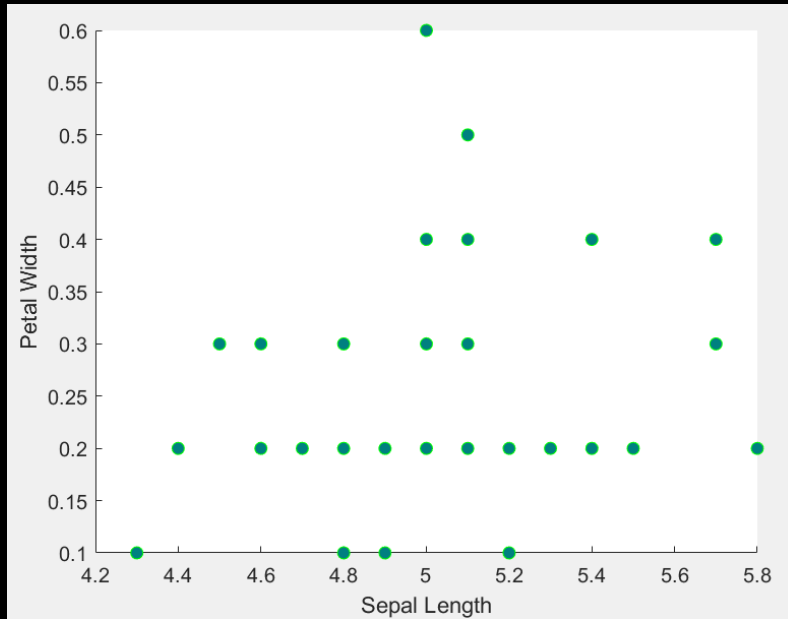
$$a_i = SL = \{5.1, 4.9 \dots, 5\}$$

$$b_i = SW = \{3.5, 3, \dots, 3.3\}$$

$$\sigma_{SL,SW}^2 = \frac{1}{n} \sum_i a_i b_i = 17.2578$$

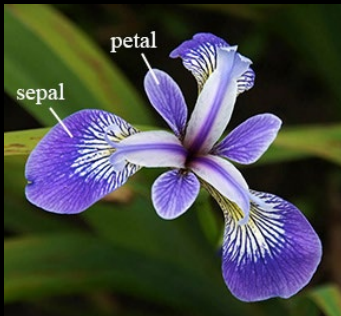
Note that in practice $n-1$ is used instead of n

Low covariance

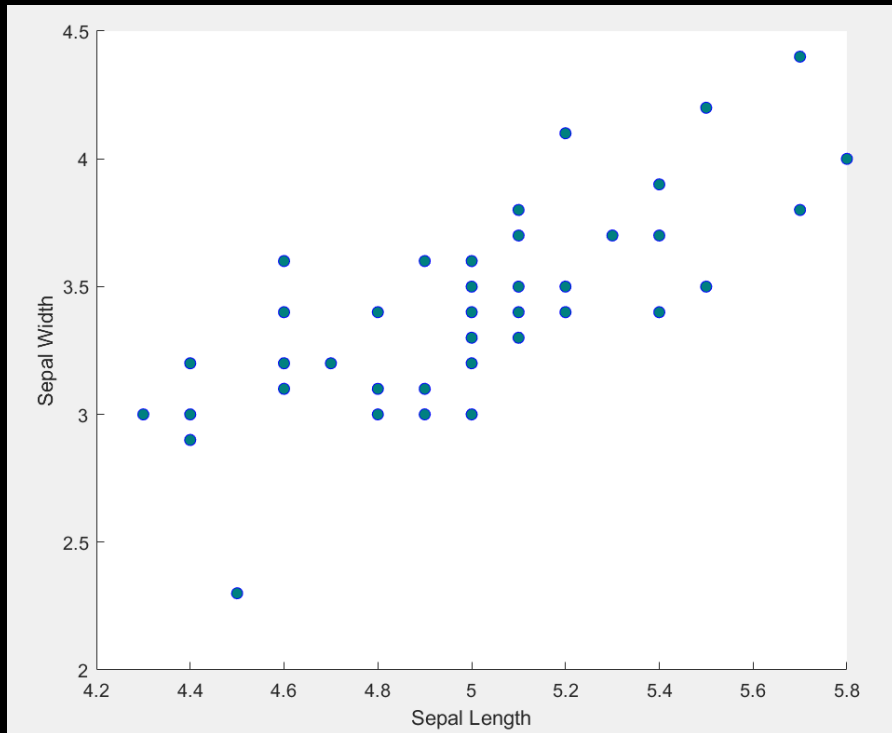


Sepal length and petal width

$$\sigma_{\text{SL,PW}}^2 = \frac{1}{n} \sum_i a_i b_i = 1.2416$$



Vector notation for covariance



Sepal length and sepal width

$$\mathbf{a} = \text{SL} = [5.1, 4.9 \dots, 5]$$

$$\mathbf{b} = \text{SW} = [3.5, 3, \dots, 3.3]$$

$$\sigma_{\text{SL}, \text{SW}}^2 = \frac{1}{n} \mathbf{a} \mathbf{b}^T$$

Matrix notation for covariance

$m \times n$ matrix ($m=4$ and $n=50$)

$$\mathbf{X} = \begin{bmatrix} \text{Sepal length}_1 & \dots & \text{Sepal length}_{50} \\ \text{Sepal width}_1 & \dots & \text{Sepal width}_{50} \\ \text{Petal length}_1 & \dots & \text{Petal length}_{50} \\ \text{Petal width}_1 & \dots & \text{Petal width}_{50} \end{bmatrix}$$

$$\mathbf{C}_\mathbf{X} \equiv \frac{1}{n} \mathbf{X} \mathbf{X}^T$$

$m \times m$ square matrix
($m=4$)

Note that in practice $n-1$ is used instead of n

Covariance matrix autopsy

$$\mathbf{C}_X \equiv \frac{1}{n} \mathbf{X} \mathbf{X}^T$$

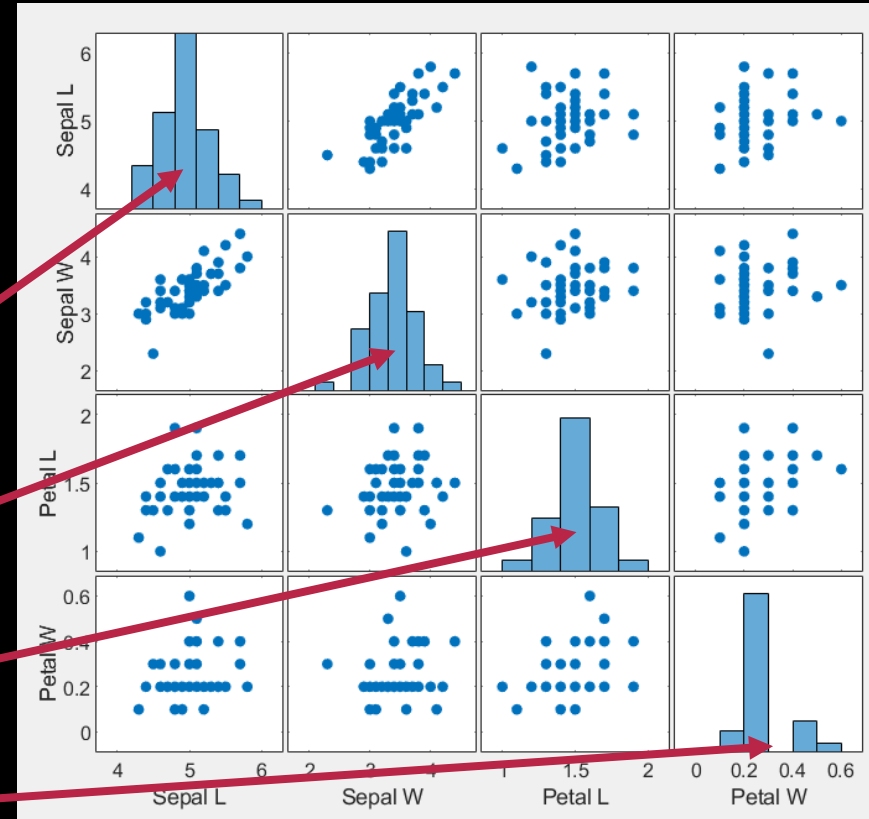
The diagonal elements are the variances

$$\sigma_{SL}^2 = 0.1242$$

$$\sigma_{SW}^2 = 0.1437$$

$$\sigma_{PL}^2 = 0.0302$$

$$\sigma_{PW}^2 = 0.0111$$



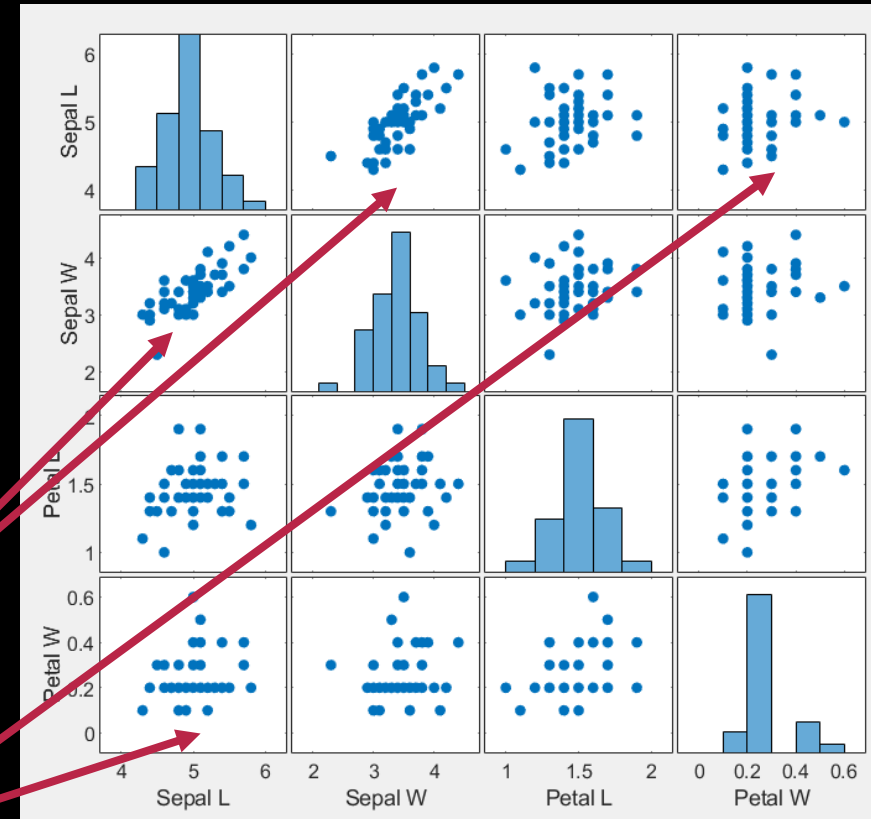
Covariance matrix autopsy II

$$\mathbf{C}_X \equiv \frac{1}{n} \mathbf{X} \mathbf{X}^T$$

The off-diagonal elements are the covariance

$$\sigma_{SL,SW}^2 = \frac{1}{n} \sum_i a_i b_i = 17.2578$$

$$\sigma_{SL,PW}^2 = \frac{1}{n} \sum_i a_i b_i = 1.2416$$

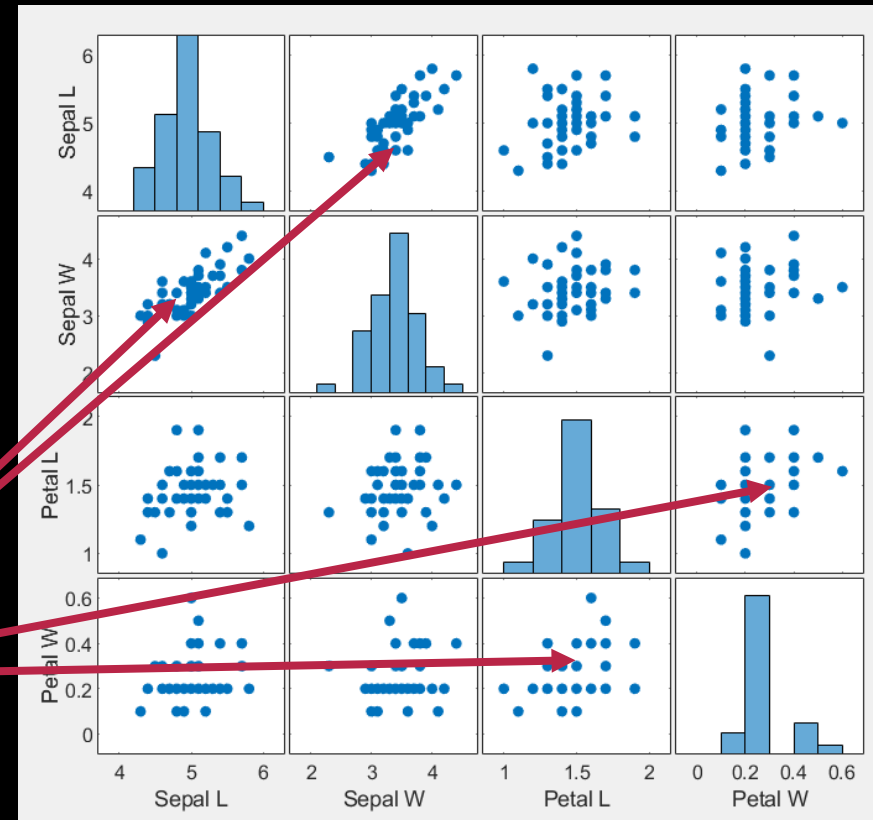


Symmetric!

Covariance matrix autopsy III

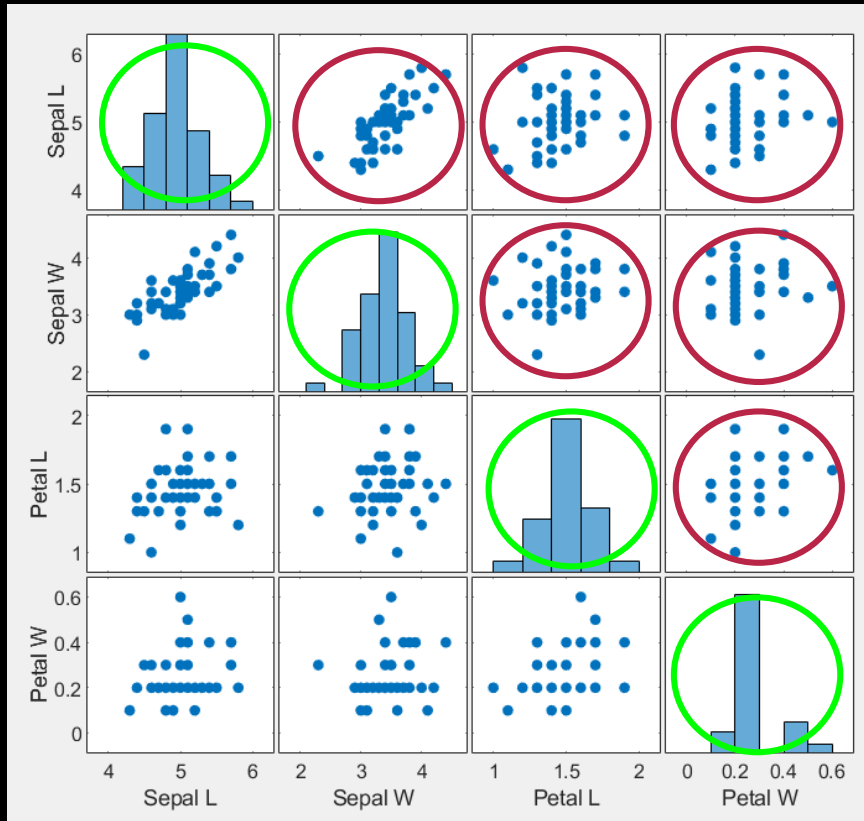
$$\mathbf{C}_X \equiv \frac{1}{n} \mathbf{X} \mathbf{X}^T$$

High redundancy



Symmetric!

Goals

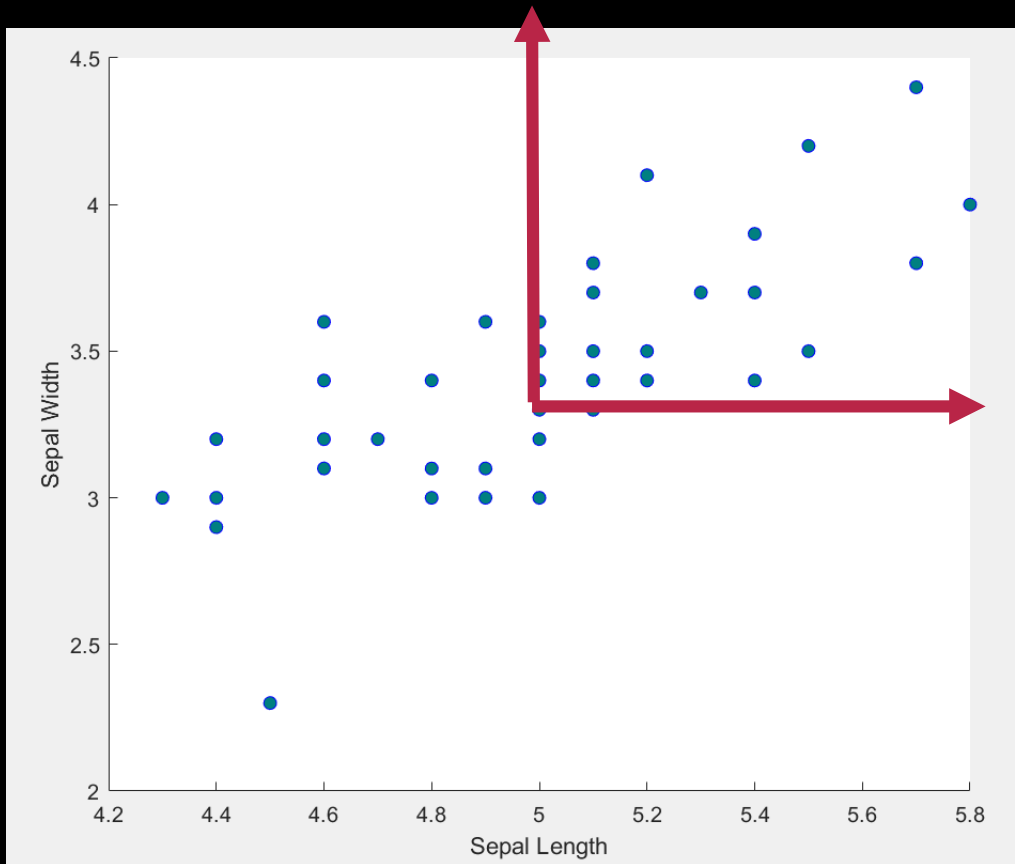


- Minimize redundancy
 - **Covariance** should be small
- Maximize signal
 - **Variance** should be large

Signal to noise ratio:

$$\text{SNR} = \frac{\sigma_{\text{signal}}^2}{\sigma_{\text{noise}}^2}$$

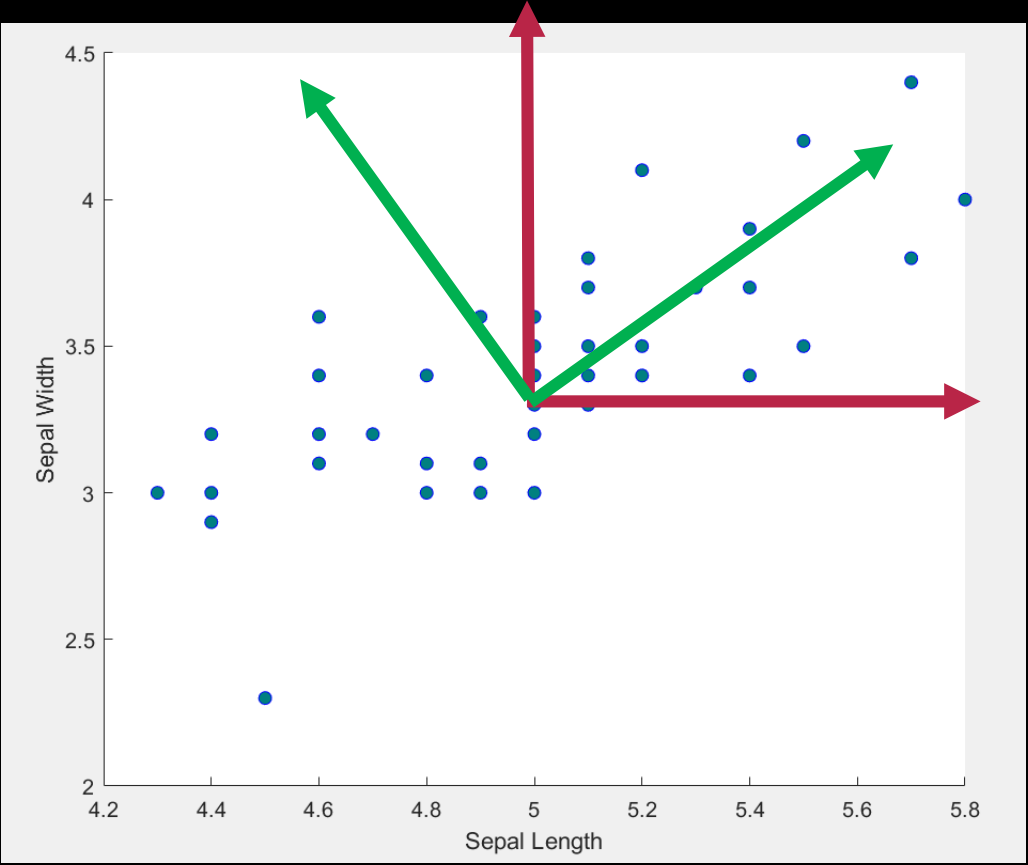
Changing basis



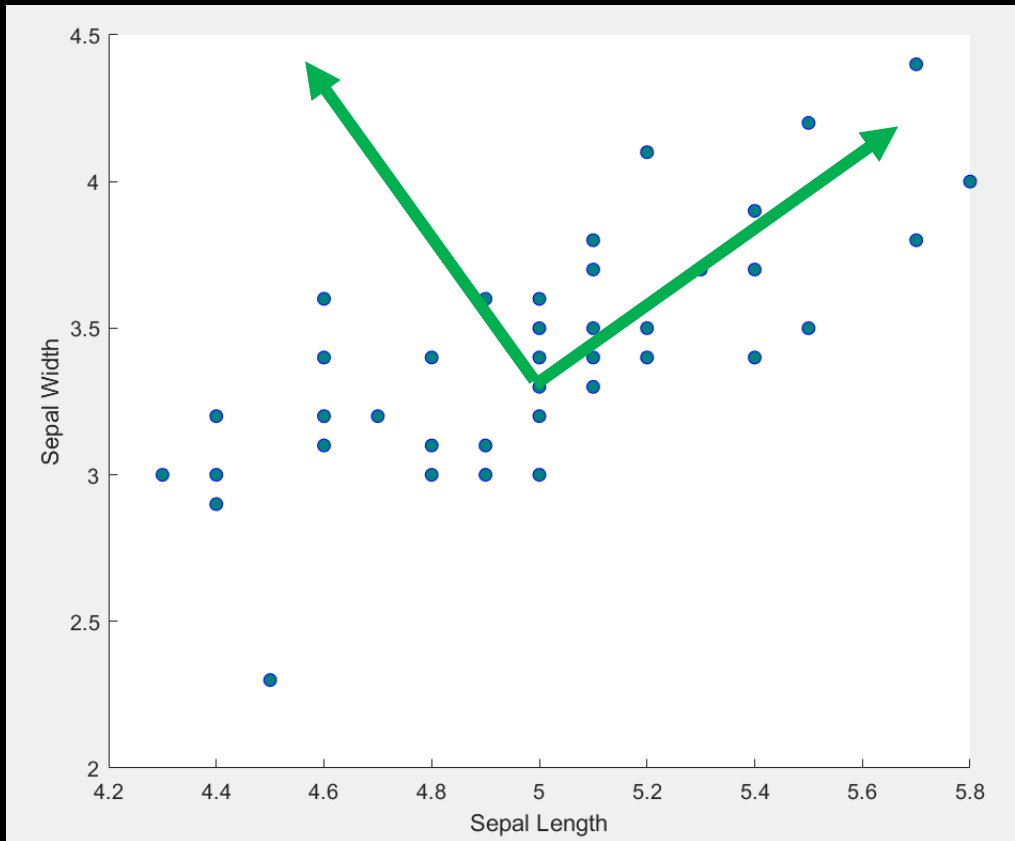
- We start by subtracting the mean
 - Centering data
- Red lines are the default basis



Changing basis

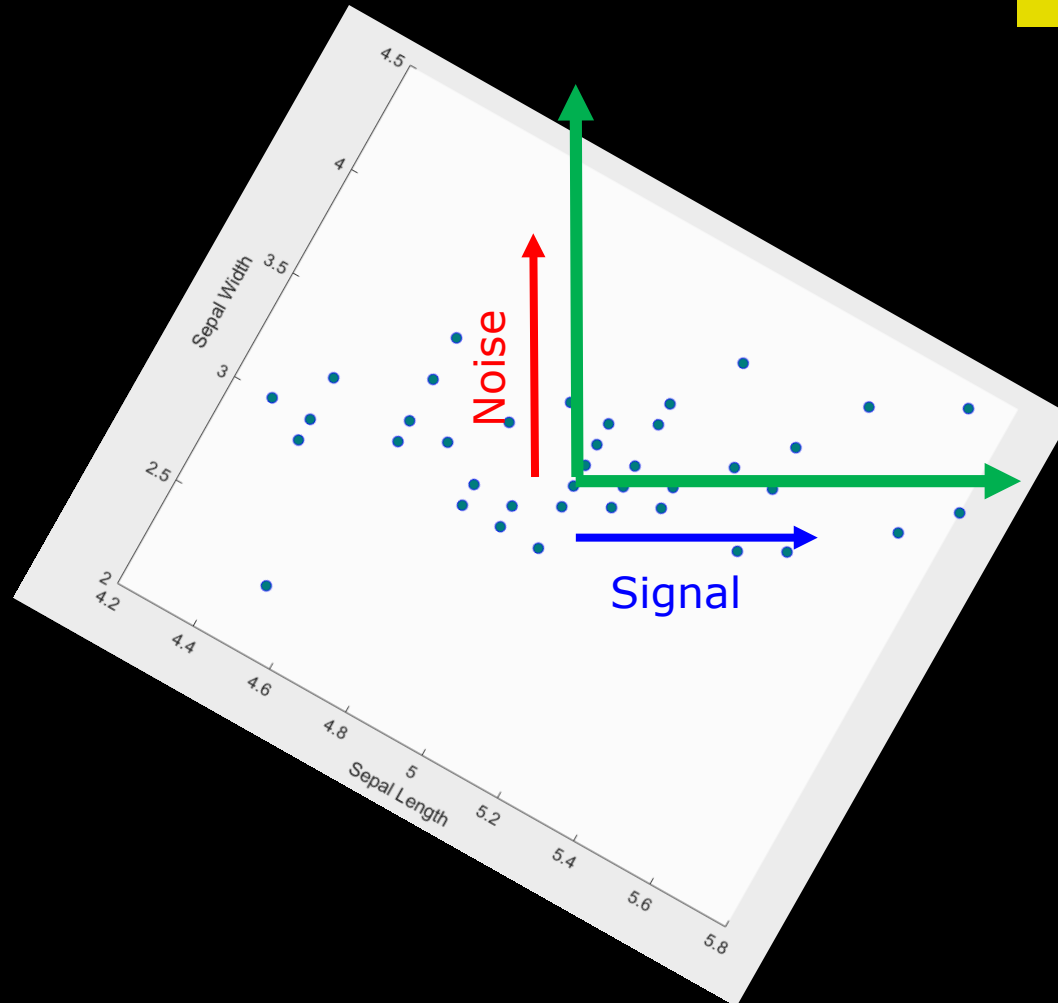


Changing basis



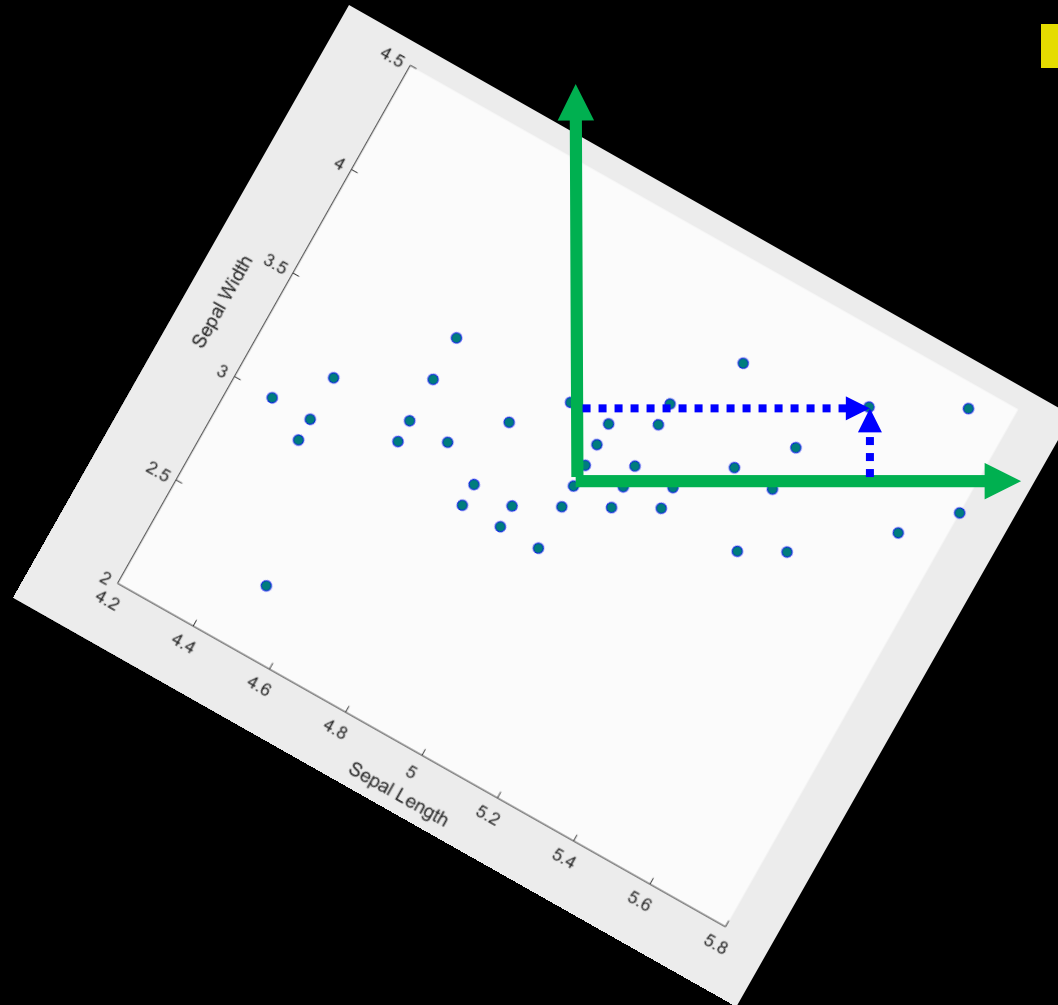
- A new basis that follows the *covariance* in the data

Changing basis



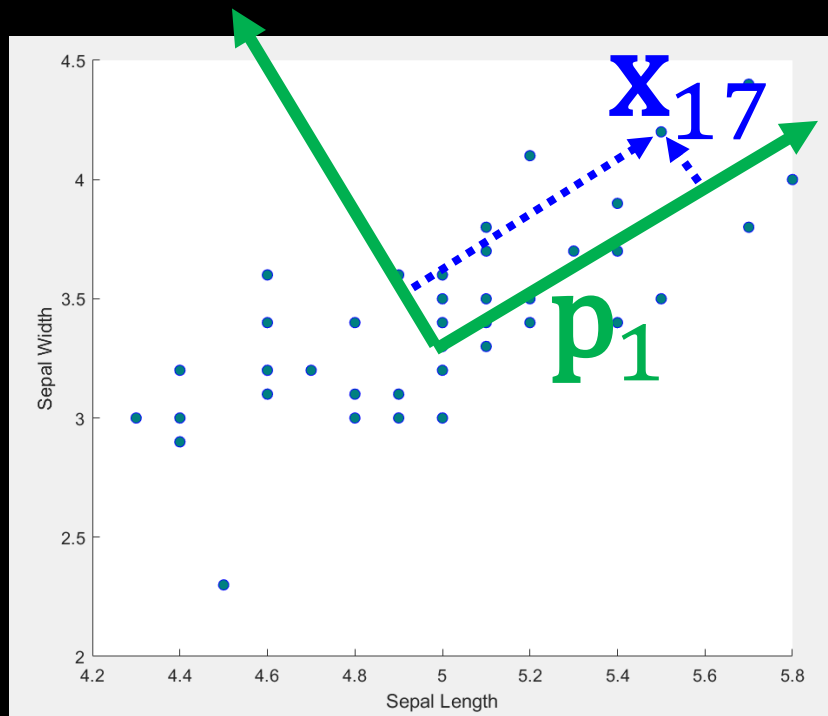
- Lets try to rotate the data – for visualisation

Changing basis



- Finding the measurement values in the new basis

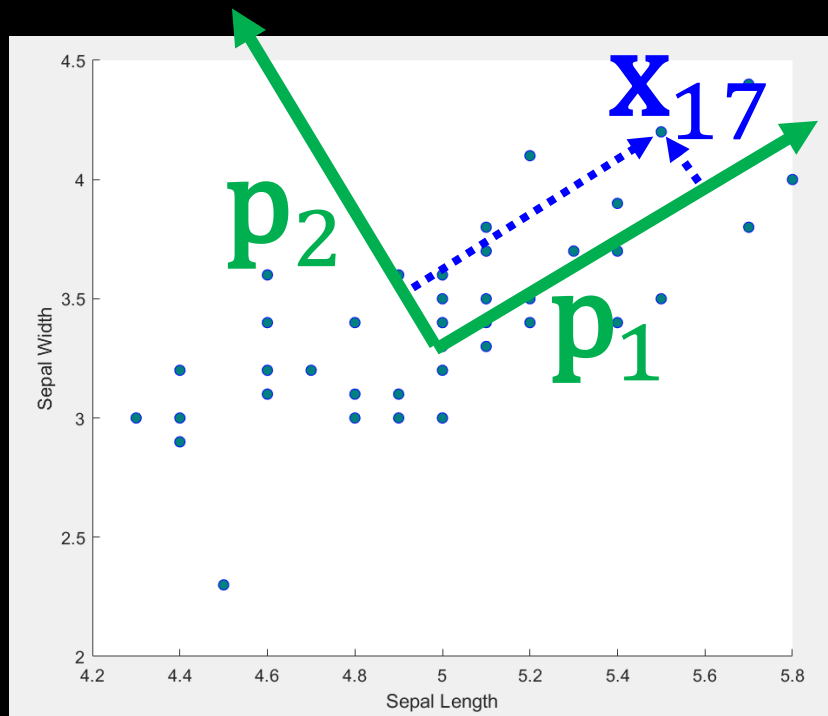
Changing basis



- The dot product projects a point down to a new axis

$$x_{17, \text{new}} = x_{17} \cdot p_1$$

Changing basis



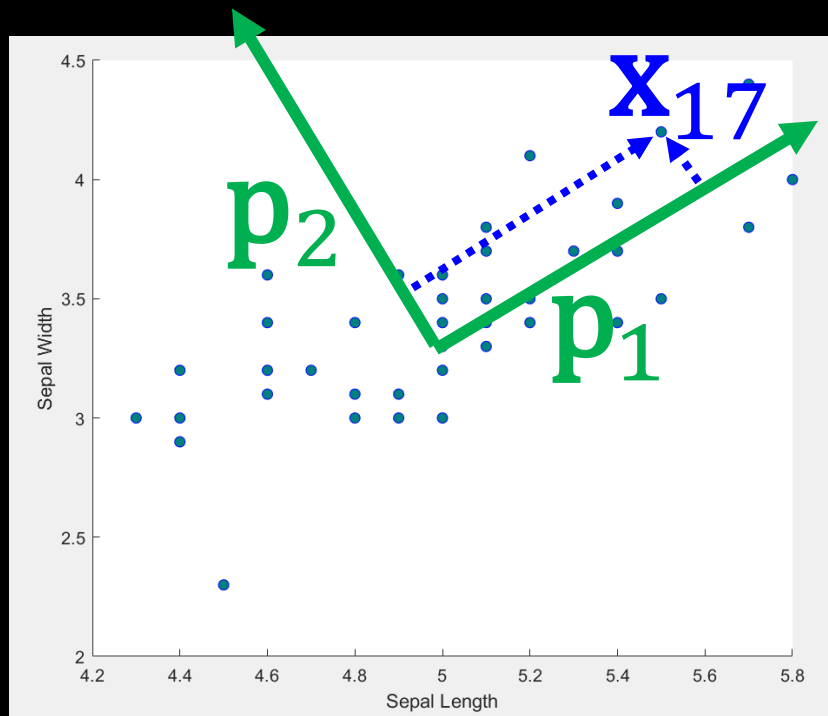
- The dot product projects a point down to a new axis

$$PX = Y$$

- p_1 and p_2 are the rows of P

$$X = \begin{bmatrix} \text{Sepal length}_1 & \dots & \text{Sepal length}_{50} \\ \text{Sepal width}_1 & \dots & \text{Sepal width}_{50} \\ \text{Petal length}_1 & \dots & \text{Petal length}_{50} \\ \text{Petal width}_1 & \dots & \text{Petal width}_{50} \end{bmatrix}$$

Changing basis

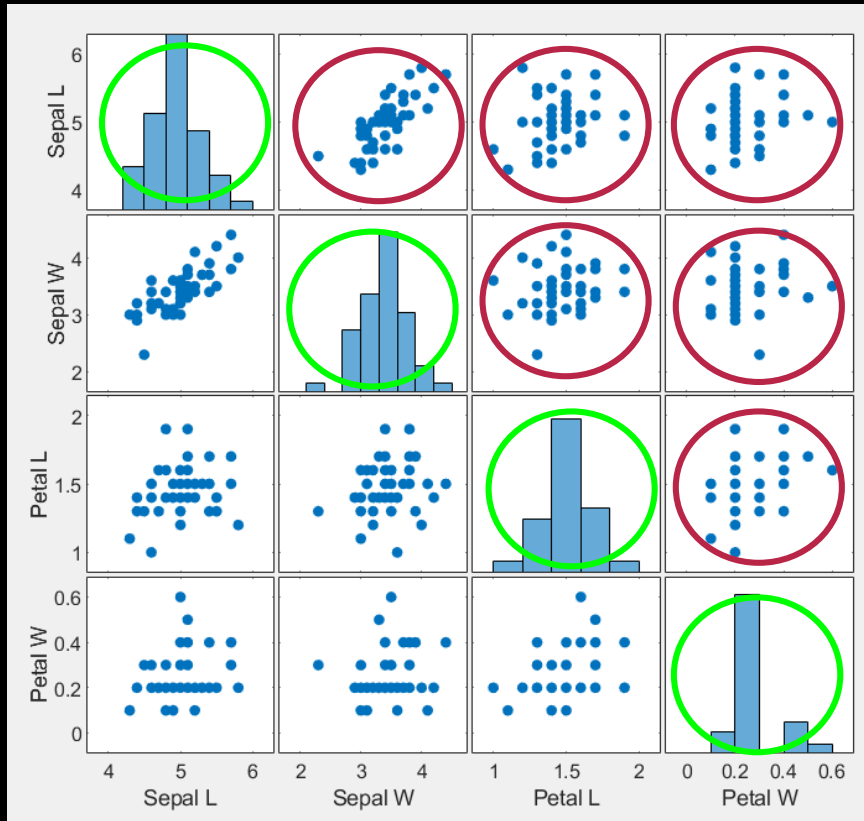


- The dot product projects a point down to a new axis

$$PX = Y$$

- Here Y contains the new coordinates/measurements per sample

Goals



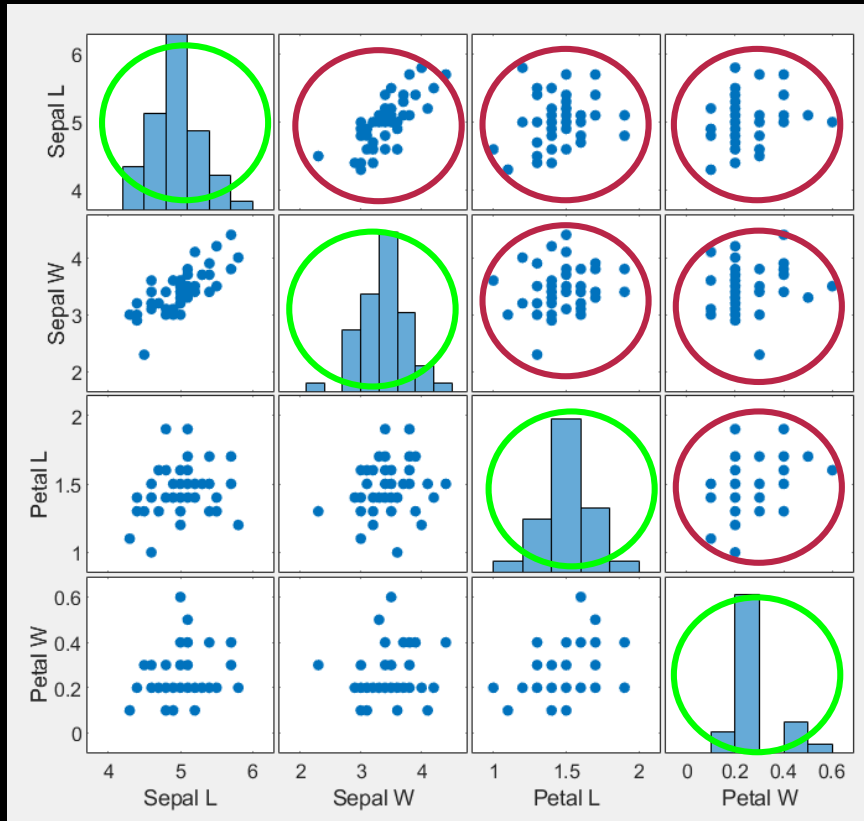
- Minimize redundancy
 - Covariance should be small
- Maximize signal
 - Variance should be large
- Transform our data
 - Rotating and scaling the basis

$$\mathbf{Y} = \mathbf{P}\mathbf{X}$$

- So it will have

$$\mathbf{C}_Y \equiv \frac{1}{n} \mathbf{Y} \mathbf{Y}^T$$

Goals



- The covariance matrix

$$\mathbf{C}_Y \equiv \frac{1}{n} \mathbf{Y} \mathbf{Y}^T$$

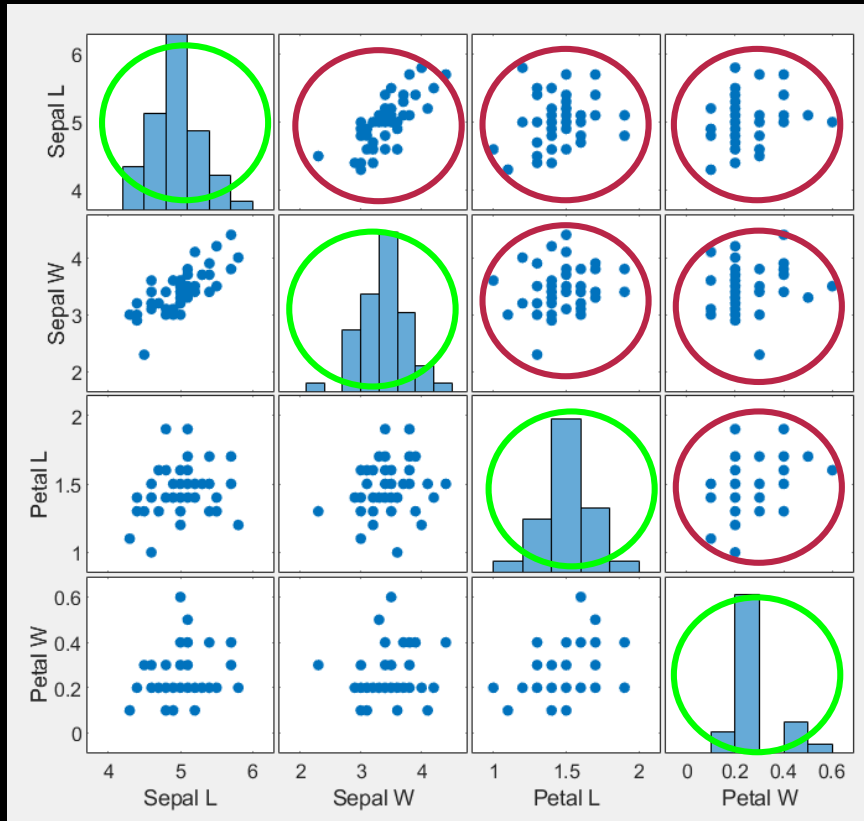
- Should be *as diagonal as possible*

- We do this by

$$\mathbf{Y} = \mathbf{P} \mathbf{X}$$

- Where **P** are the principal components

Computing the principal components

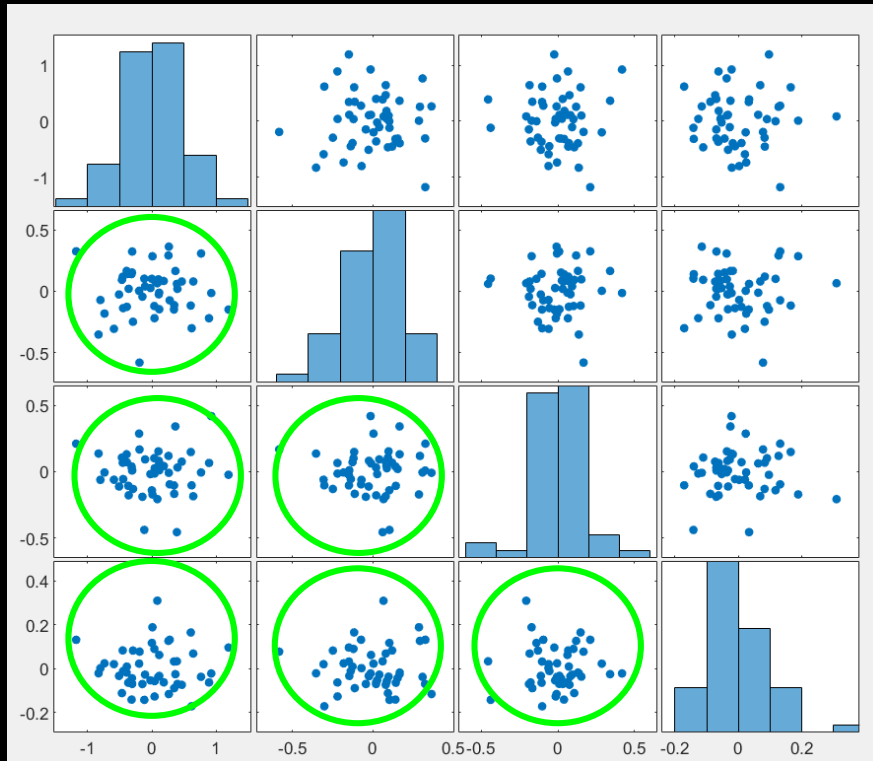


- The Principal Components of \mathbf{X} are the **eigenvectors** of

$$\mathbf{C}_\mathbf{X} \equiv \frac{1}{n} \mathbf{X} \mathbf{X}^T$$

- The i 'th diagonal value of $\mathbf{C}_\mathbf{Y}$ is the variance along principal component number i

New covariance matrix for Iris data



Covariance: 0

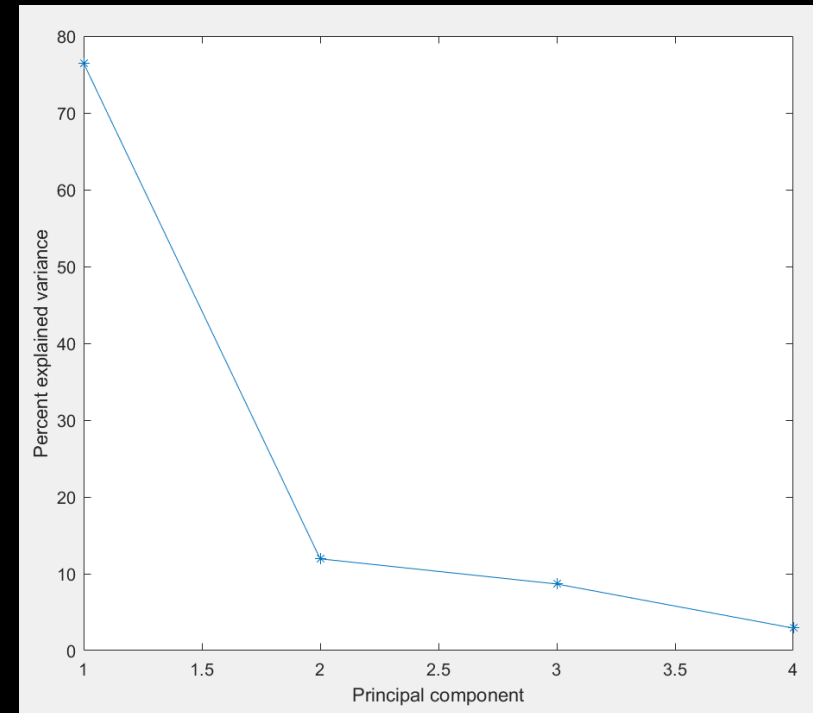
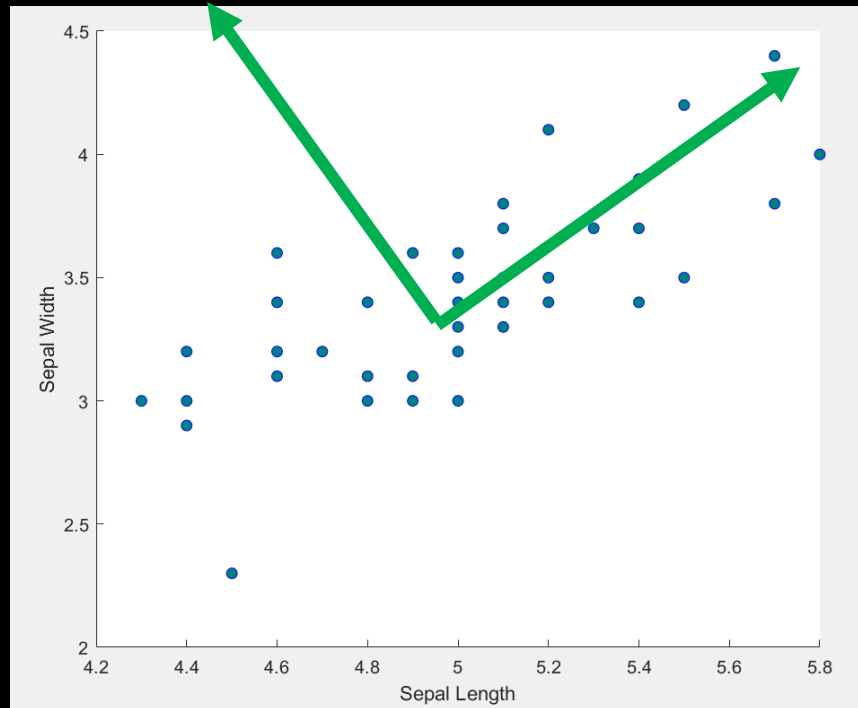
- The principal component are found and

$$\mathbf{Y} = \mathbf{P}\mathbf{X}$$

- With the covariance matrix

$$\mathbf{C}_Y \equiv \frac{1}{n} \mathbf{Y}\mathbf{Y}^T$$

Explained variance



One component explains 75% of the total variation – so for each flower we can have one number that explains 75% percent of the 4 measurements!

What can we use it for?

■ Classification





Based on one value instead of 4



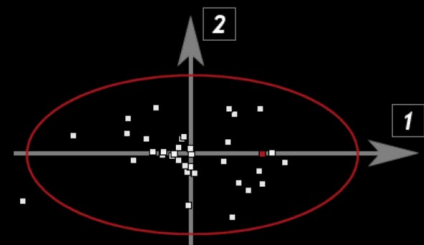
What can we use it for?

- Many more examples in the course





generate faces by adjusting sliders [1]-[6]



1

2

3

4


5

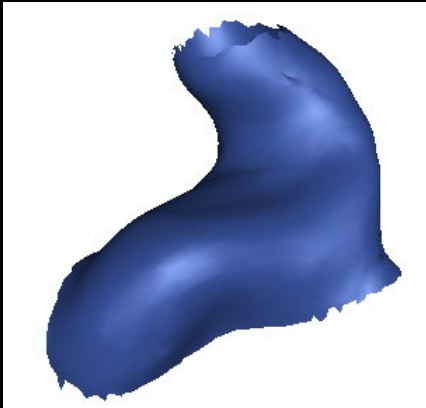
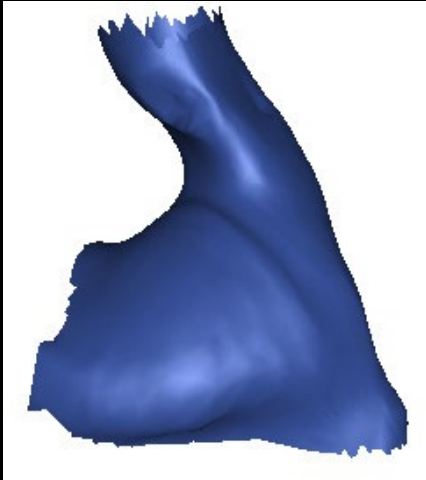
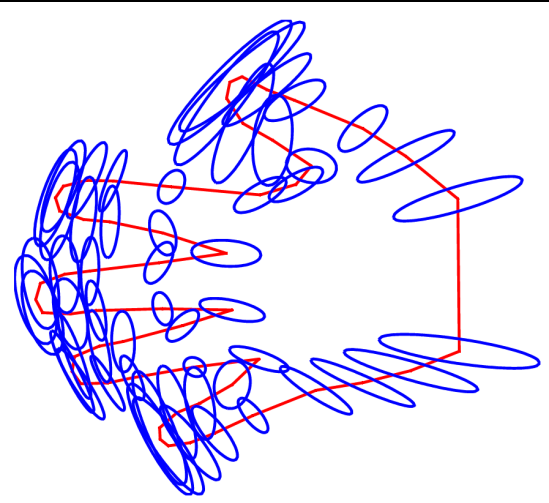
6

demo

reset

help





Final note – practical estimation of covariance matrix

$$\mathbf{C}_{\mathbf{X}} \equiv \frac{1}{n} \mathbf{X} \mathbf{X}^T$$

In practice $n-1$ is used instead of n for exercises and in the exam.

$$\mathbf{C}_{\mathbf{X}} \equiv \frac{1}{n-1} \mathbf{X} \mathbf{X}^T$$