# Principle Component Analysis

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# Outline

- Introduction
- Objective
- Coordinate System
- PCA Visualization
- Steps of Principle Component Analysis
- Variance & Covariance
- Eigenvector & Eigenvalue
- Conclusion

# Introduction

PCA (Principle Component Analysis) is defined as an orthogonal linear transformation that transforms the data to a new coordinate system such that the greatest variance comes to lie on the first coordinate, the second greatest variance on the second coordinate and so on.

# Objective

- Principal component analysis (PCA) is a way to reduce data dimensionality
- PCA projects high dimensional data to a lower dimension
- PCA projects the data in the least square sense– it captures big (principal) variability in the data and ignores small variability

# Philosophy of PCA

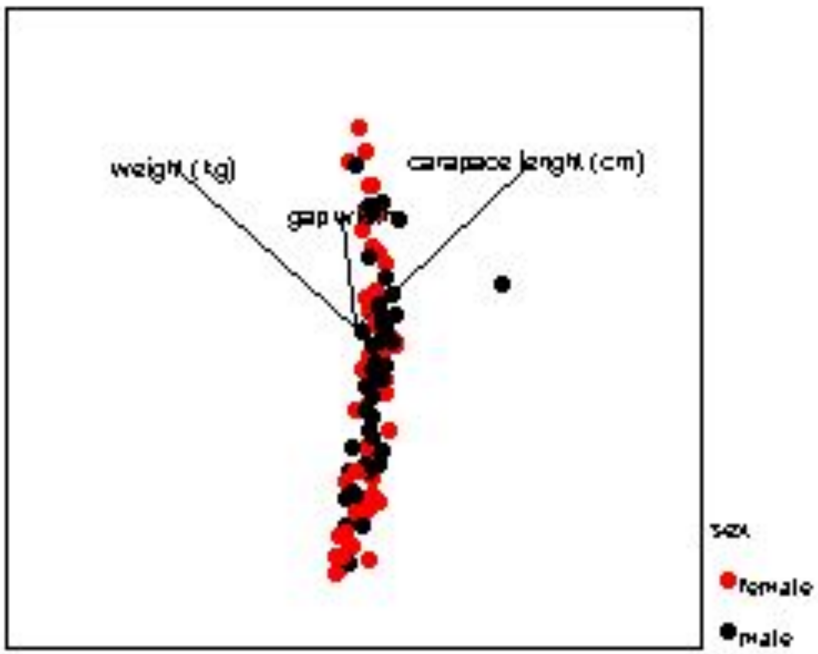
- Introduced by Pearson (1901) and Hotelling (1933) to describe the variation in a set of multivariate data in terms of a set of uncorrelated variables

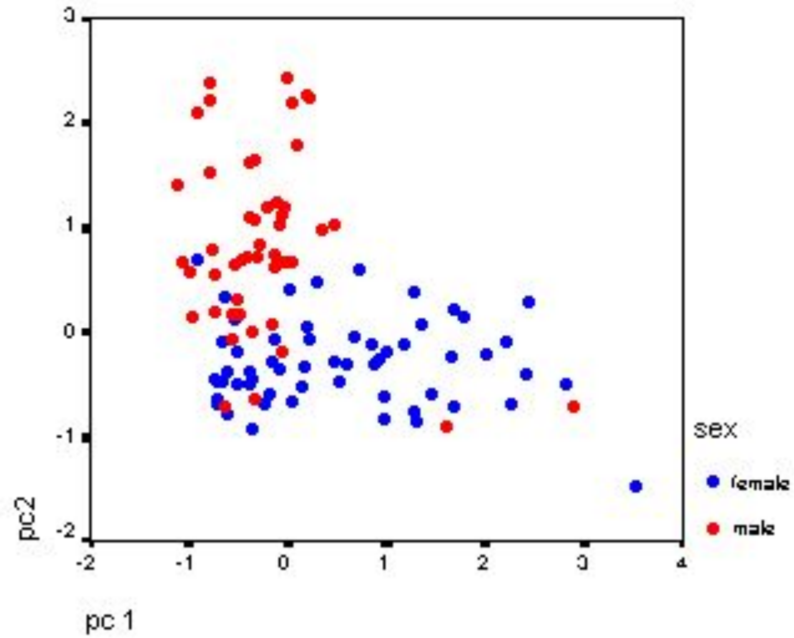
- We typically have a data matrix of $n$ observations on $p$ correlated variables $x_1, x_2, \ldots x_p$

- PCA looks for a transformation of the $x_i$ into $p$ new variables $y_i$ that are uncorrelated

# Data set

| case | ht ($x_1$) | wt($x_2$) | age($x_3$) | sbp($x_4$) | heart rate ($x_5$) |
|---|---|---|---|---|---|
| 1 | 175 | 1225 | 25 | 117 | 56 |
| 2 | 156 | 1050 | 31 | 122 | 63 |
| n | 202 | 1350 | 58 | 154 | 67 |



# Principal Component Analysis

- Each Coordinate in Principle Component Analysis is called Principle Component.

$$C_i = b_{i1}\,(x_1) + b_{i2}\,(x_2) + \ldots + b_{in}(x_n)$$

where, $C_i$ is the $i^{th}$ principle component, $b_{ij}$ is the regression coefficient for observed variable j for the principle component i and $x_i$ are the variables/dimensions.

# Principal Component Analysis[cont..]

From $k$ original variables: $x_1,x_2,...,x_k$:

Produce $k$ new variables: $y_1,y_2,...,y_k$:

$$
\begin{aligned}
y_1 &= a_{11}x_1 + a_{12}x_2 + ... + a_{1k}x_k \\
y_2 &= a_{21}x_1 + a_{22}x_2 + ... + a_{2k}x_k \\
&... \\
y_k &= a_{k1}x_1 + a_{k2}x_2 + ... + a_{kk}x_k
\end{aligned}
$$

# Principal Component Analysis[cont..]

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# Principal Component Analysis[cont..]

From $k$ original variables: $x_1, x_2, \ldots, x_k$:

Produce $k$ new variables: $y_1, y_2, \ldots, y_k$:

$$y_1 = a_{11}x_1 + a_{12}x_2 + \ldots + a_{1k}x_k$$

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$$\ldots$$

$$y_k = a_{k1}x_1 + a_{k2}x_2 + \ldots + a_{kk}x_k$$

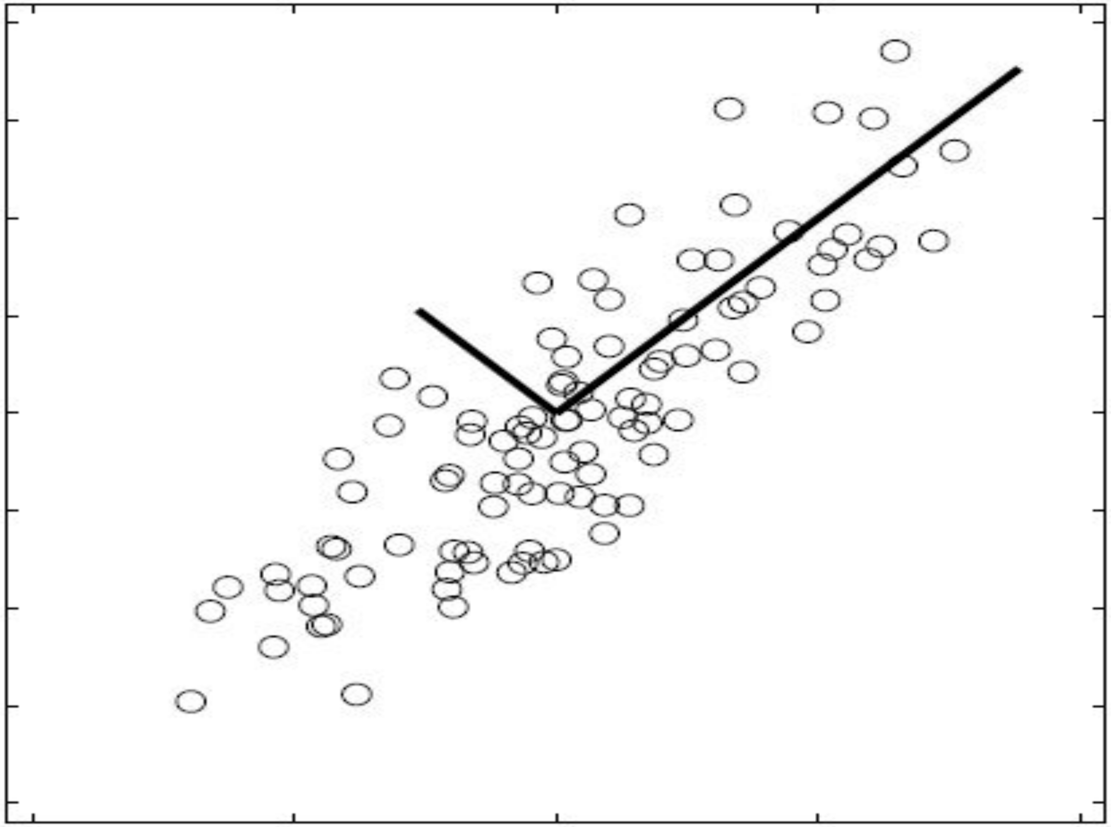
*such that:*

$y_k$'s are uncorrelated (orthogonal)

$y_1$ explains as much as possible of original variance in data set

$y_2$ explains as much as possible of remaining variance etc.

# PCA: Visually



Data points are represented in a rotated **orthogonal** coordinate system: the origin is the **mean** of the data points and the axes are provided by the **eigenvectors**

# Steps to Find Principle Component

1. Adjust the dataset to zero mean dataset.
2. Find the Covariance Matrix $M$
3. Calculate the normalized Eigenvectors and Eigenvalues of $M$
4. Sort the Eigenvectors according to Eigenvalues from highest to lowest

# Eigenvector and Principle Component

- It turns out that the Eigenvectors of covariance matrix of the data set are the principle components of the data set.

- Eigenvector with the highest eigenvalue is first principle component and with the $2^{nd}$ highest eigenvalue is the second principle component and so on

# Example

AdjustedData Set=Original Data-Mean

| X | Y |
|---|---|
| 2.5 | 2.4 |
| 0.5 | 0.7 |
| 2.2 | 2.9 |
| 1.9 | 2.2 |
| 3.1 | 3.0 |
| 2.3 | 2.7 |
| 2 | 1.6 |
| 1 | 1.1 |
| 1.5 | 1.6 |
| 1.1 | 0.9 |

Original Data set

| X | Y |
|---|---|
| 0.69 | 0.49 |
| -1.31 | -1.21 |
| 0.39 | 0.99 |
| 0.09 | 0.29 |
| 1.29 | 1.09 |
| 0.49 | 0.79 |
| 0.19 | -0.31 |
| -0.81 | -0.81 |
| -0.31 | -0.31 |
| -0.71 | -1.01 |

Adjusted Data Set

# Variance & Covariance

- The **variance** is a measure of how far a set of numbers is spread out.
- The equation of variance is

$$Var(x) = \frac{\sum_{i=1}^{n}\left(X_i - \overline{X}\right)\left(X_i - \overline{X}\right)}{n-1}$$

# Variance & Covariance (cont..)

- Covariance measure how much to random variable change together.

Equation of Covariance:

$$Cov(x,y) = \frac{\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})}{n-1}$$

# Covariance Matrix

A covariance matrix n*n matrix where each element can be defined as

$$M_{ij} = \text{cov}(i, j)$$

A Covariance Matrix on 2-Dimensional Data Set:

$$M = \begin{bmatrix} Cov(x,x) & Cov(x,y) \\ Cov(y,x) & Cov(y,y) \end{bmatrix}$$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# Covariance Matrix(Cont...)

$$M = \begin{bmatrix} 0.616555556 & 0.615444444 \\ 0.615444444 & 0.716555556 \end{bmatrix}$$

# Eigenvector & Eigenvalue

- The **eigenvectors** of a square matrix *A* are the non-zero vectors *x* such that, after being multiplied by the matrix, remain parallel to the original vector.

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

# Eigenvector & Eigenvalue(cont..)

- For each Eigenvector, the corresponding **Eigenvalue** is the factor by which the eigenvector is scaled when multiplied by the matrix.
- $$\begin{bmatrix} 2 & 1 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} 3 \\ -3 \end{bmatrix} = 1. \begin{bmatrix} 3 \\ -3 \end{bmatrix}$$

# Eigenvector & Eigenvalue(cont..)

- The vector $x$ is an eigenvector of the matrix $A$ with eigenvalue λ (lambda) if the following equation holds:

$$Ax = \lambda x$$

$$or, Ax - \lambda x = 0$$

$$or, (A - \lambda I)x = 0$$

# Eigenvector & Eigenvalue(cont..)

Calculating Eigenvalues

$$\left|A - \lambda I\right| = 0$$

Calculating Eigenvector

$$\left(A - \lambda I\right)x = 0$$

# Example…

Suppose A is a matrix

$$A = \begin{bmatrix} 1 & 0 & -1 \\ 1 & 2 & 1 \\ 2 & 2 & 3 \end{bmatrix}$$

Finding Eigenvalue using $|A - \lambda I| = 0$

$$\begin{bmatrix} 1-\lambda & 0 & -1 \\ 1 & 2-\lambda & 1 \\ 2 & 2 & 3-\lambda \end{bmatrix} = 0$$

or, $(\lambda - 1)(\lambda - 2)(\lambda - 3) = 0$

$\Rightarrow \lambda = 1,2,3$

# Example…

Finding Eigenvector using $(A-\lambda I)x = 0$

For ,λ=1

$$\begin{bmatrix} 0 & 0 & -1 \\ 1 & 1 & 1 \\ 2 & 2 & 2 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$$

So, $-z = 0$

$x + y + z = 0$

Let, x=k and y=-k

Eigenvector $x_1$ is

$$\begin{bmatrix} k \\ -k \\ 0 \end{bmatrix} = \begin{bmatrix} 1 \\ -1 \\ 0 \end{bmatrix}$$

# Example…

For λ=2,

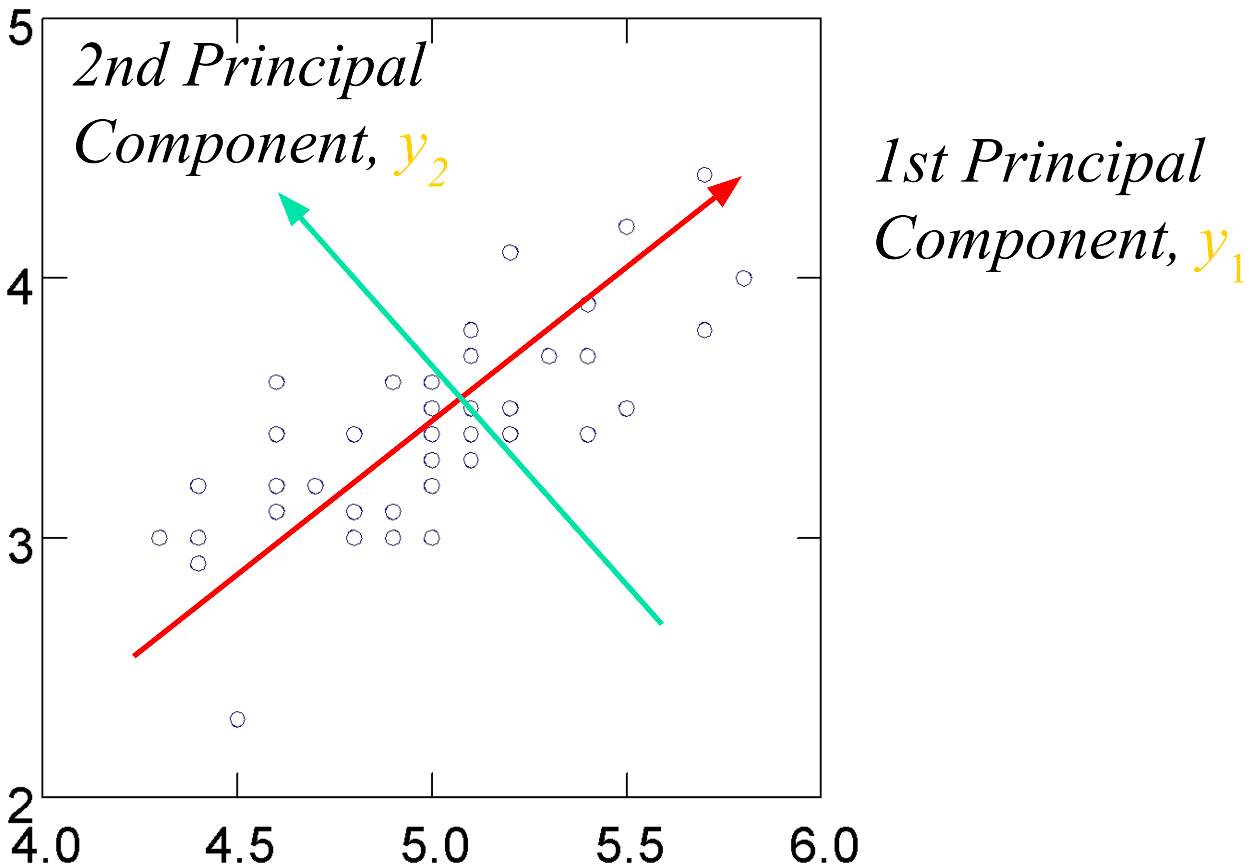
$$\text{Eigenvector } x_2 = \begin{bmatrix} 2 \\ -1 \\ 2 \end{bmatrix}$$

For λ=3,

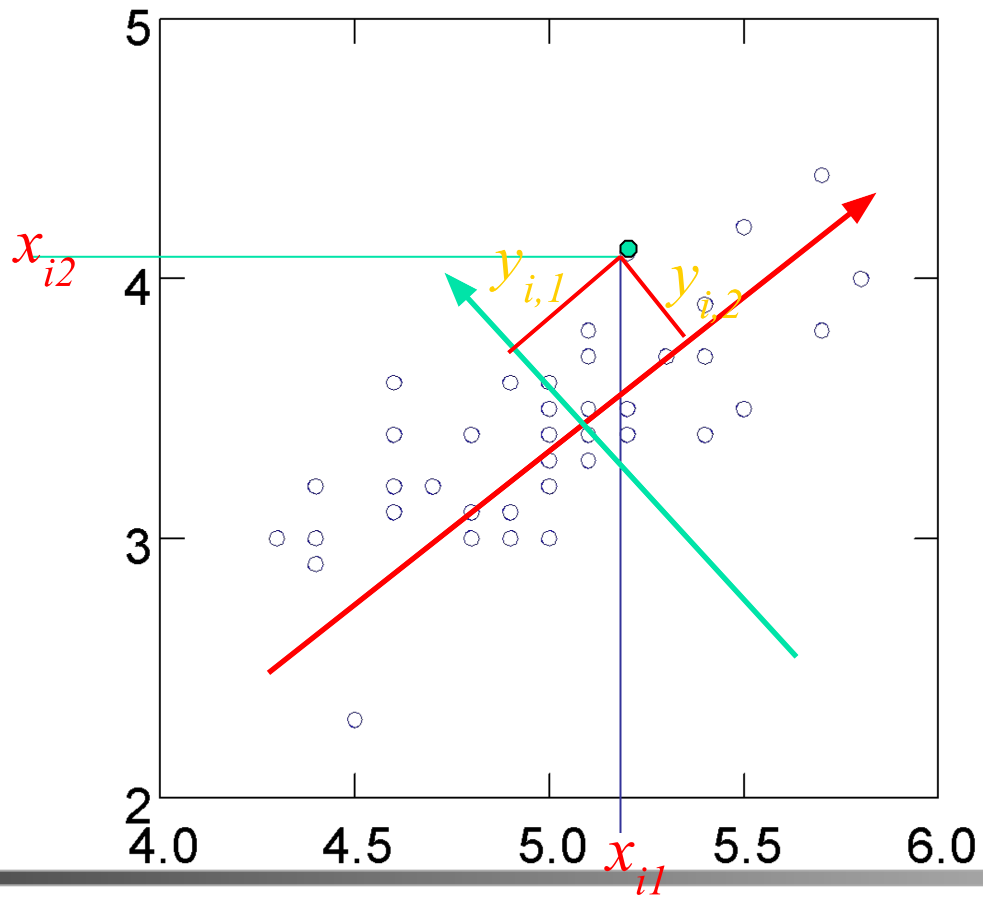
$$\text{Eigenvector } x_3 = \begin{bmatrix} 1 \\ -1 \\ -2 \end{bmatrix}$$

$$\text{So, Normalized Eigenvector } x = \begin{bmatrix} 1 & 2 & 1 \\ -1 & -1 & -1 \\ 0 & 2 & -2 \end{bmatrix}$$

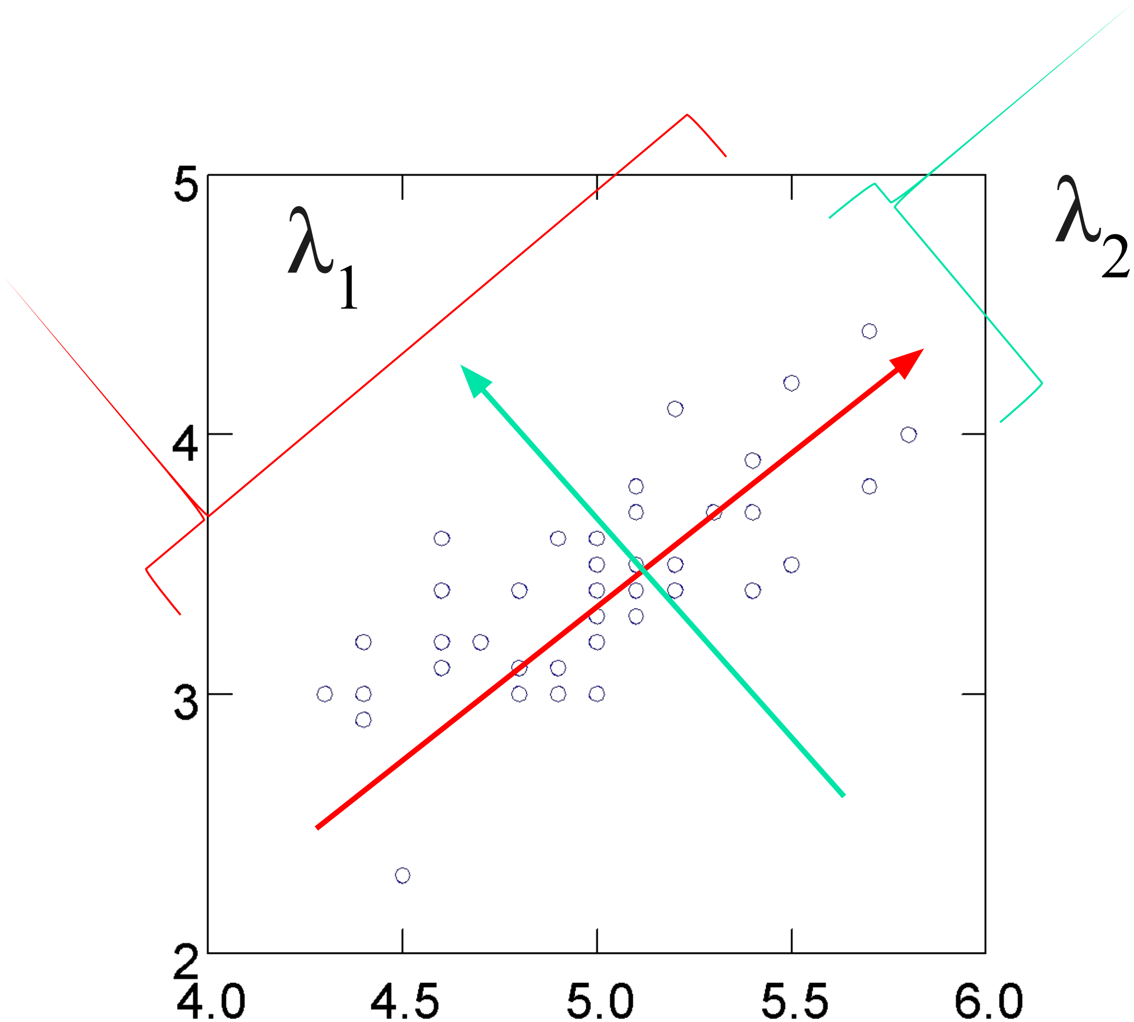
# PCA Presentation



# PCA Scores



# PCA Eigenvalues



# Application

- Uses:
  - Data Visualization
  - Data Reduction
  - Data Classification
  - Trend Analysis
  - Factor Analysis
  - Noise Reduction

- Examples:
  - How many unique “sub-sets” are in the sample?
  - How are they similar / different?
  - What are the underlying factors that influence the samples?
  - Which time / temporal trends are (anti)correlated?
  - Which measurements are needed to differentiate?
  - How to best present what is “interesting”?
  - Which “sub-set” does this new sample rightfully belong?

Thanks to All