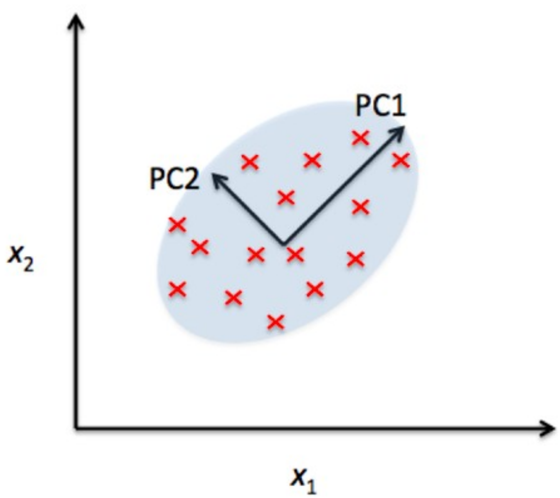
*Blockkurs:*
**Introduction to Machine Learning for Psychologists**

# Multidimensional Data and Dimensionality Reduction




Yannick Rothacher

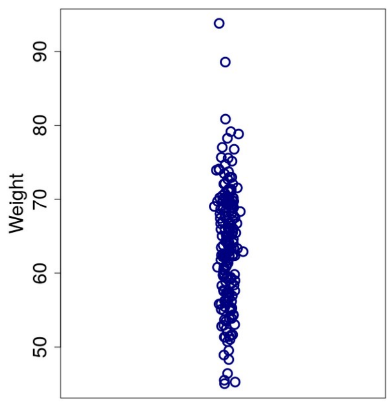
*Zürich, FS2025*

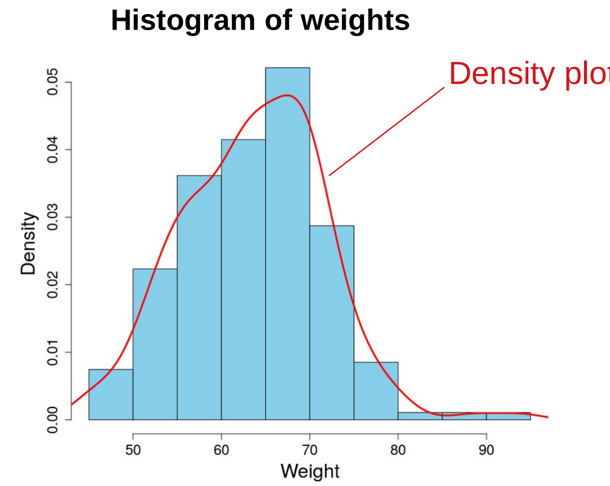
University of Zurich[UZH]

# Univariate data set

- This is the most simple data set possible

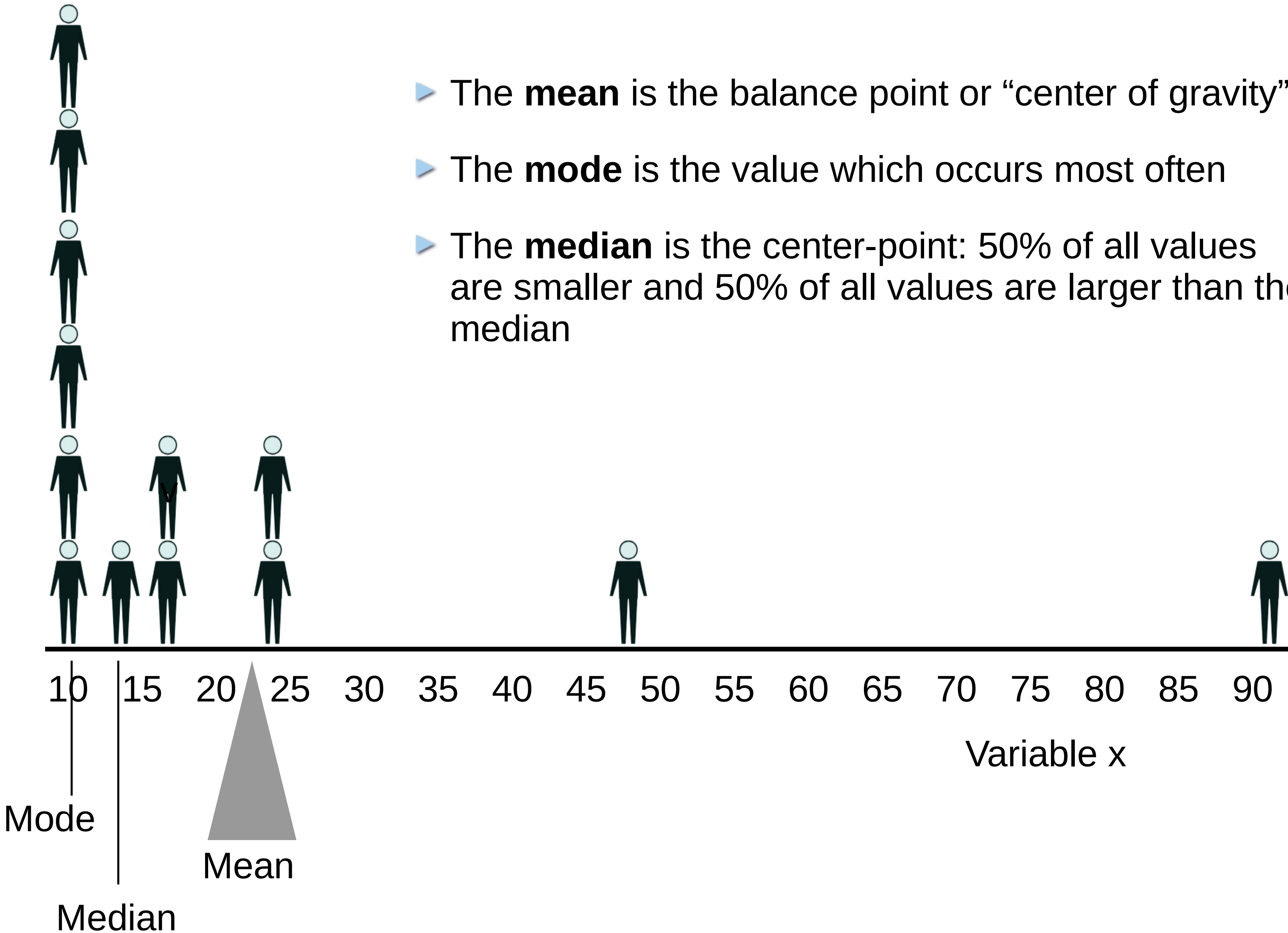
| Participant | Weight (kg) |
|---|---|
| S1 | 64 |
| S2 | 80 |
| S3 | 55 |
| S4 | 84 |
| ... | ... |



# Recap: Descriptive statistics

- The **mean** is the balance point or “center of gravity”
- The **mode** is the value which occurs most often
- The **median** is the center-point: 50% of all values are smaller and 50% of all values are larger than the median



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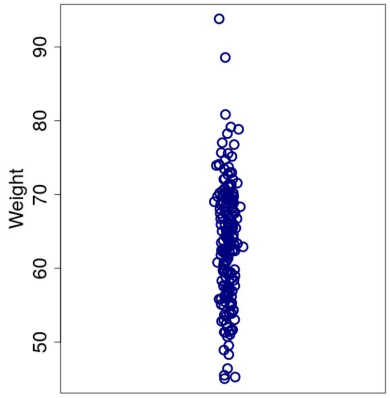


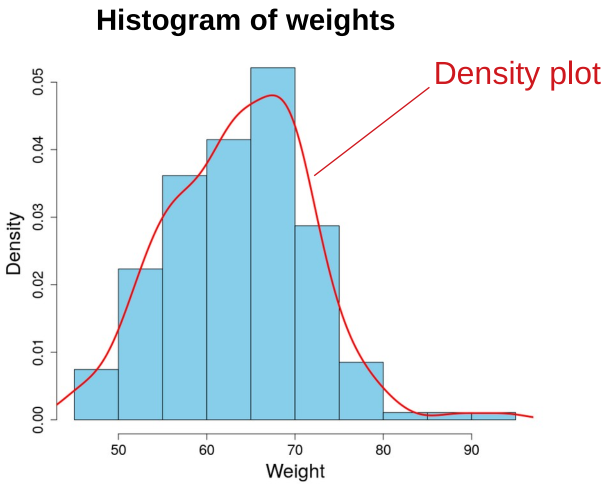

# Univariate data set

- Descriptive statistics

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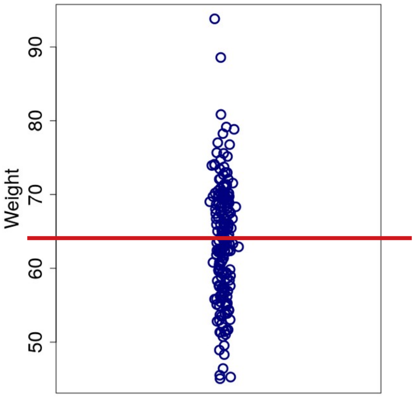


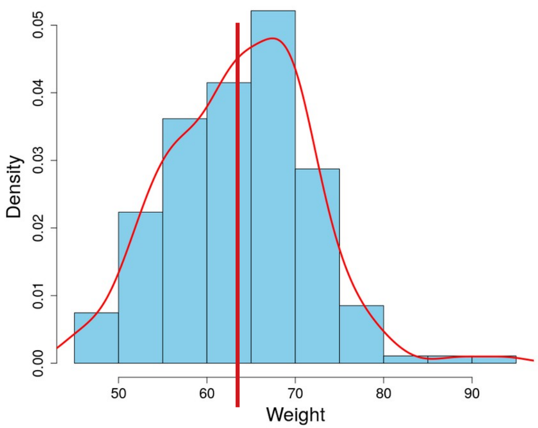


**Mean**: *"Average of a distribution"* $\bar{x} = \frac{\sum x_i}{n}$ 63.7 kg

# Univariate data set

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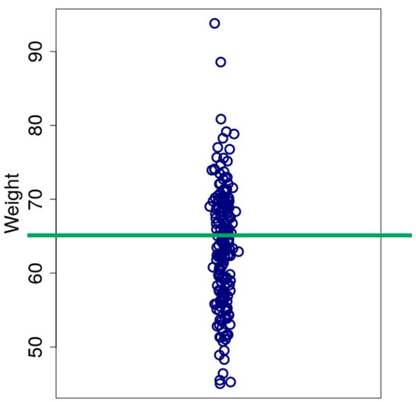


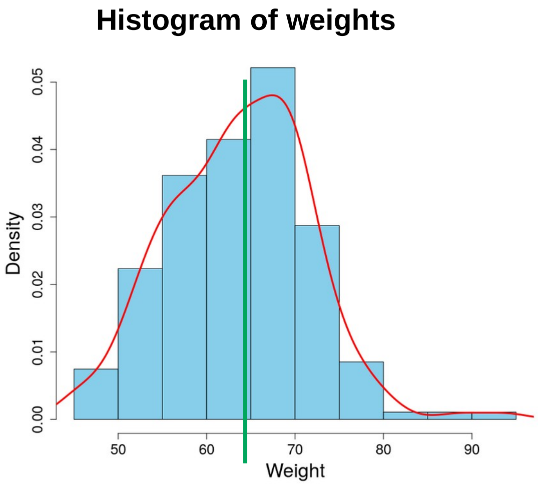


**Mean**: *"Average of a distribution"* $\bar{x} = \frac{\sum x_i}{n}$ 63.7 kg

**Median**: *"Midpoint of a distribution"* 63.9 kg

# Univariate data set

- Descriptive statistics

| Participant | Weight (kg) |
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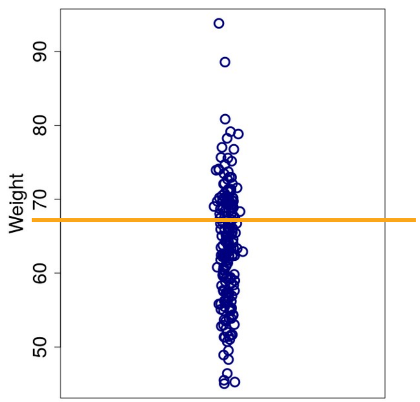


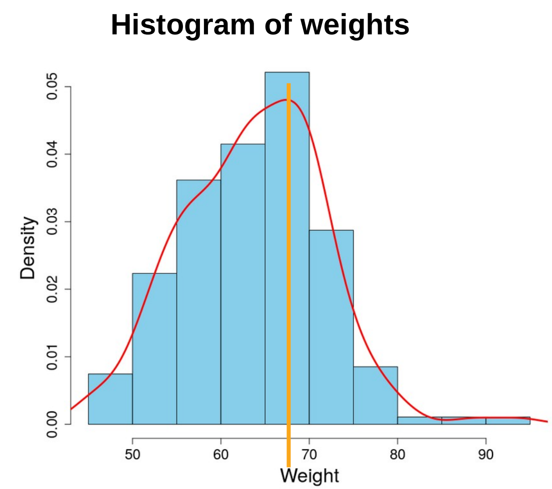


**Mean**: *"Average of a distribution"* $\bar{x} = \frac{\sum x_i}{n}$ 63.7 kg

**Median**: *"Midpoint of a distribution"* 63.9 kg

**Mode**: *"The peak(s) of a distribution"* 67.4 kg

# Univariate data set

- Descriptive statistics

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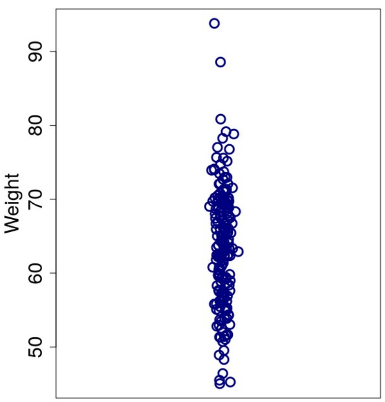
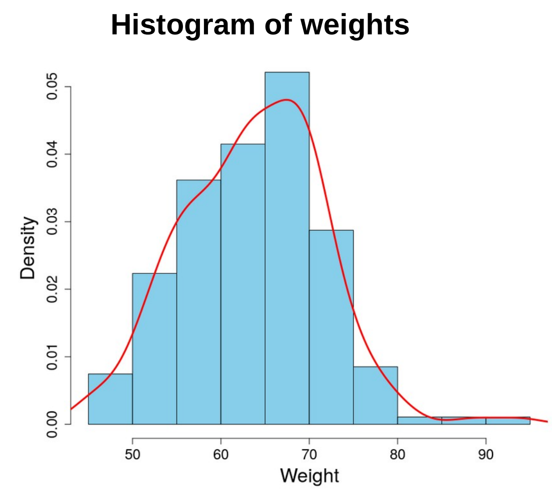



**Mean**: *"Average of a distribution"* $\bar{x} = \frac{\sum x_i}{n}$ 63.7 kg

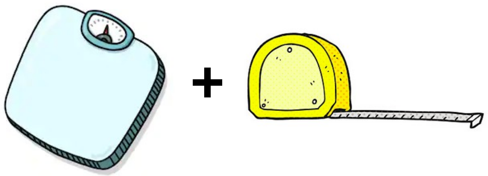
**Median**: *"Midpoint of a distribution"* 63.9 kg

**Mode**: *"The peak(s) of a distribution"* 67.4 kg

**Standard deviation**: *"Spread of distribution"* 7.9 kg

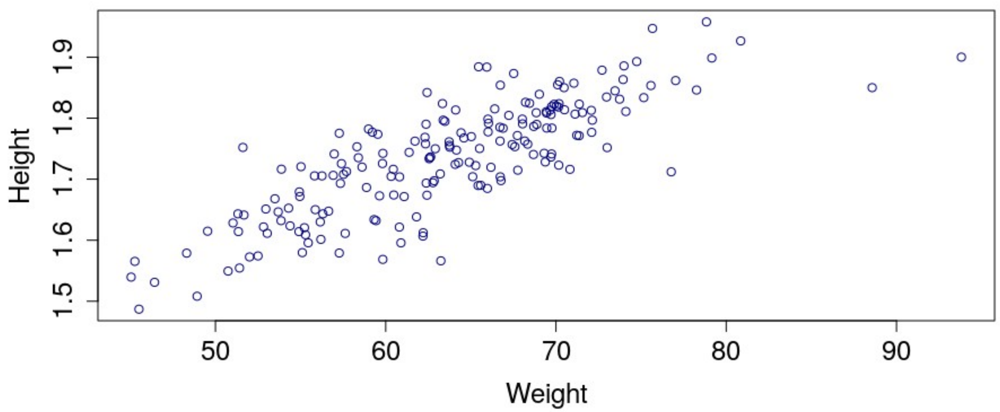
$$s = \sqrt{\frac{\sum (x_i - \bar{x})^2}{n-1}}$$ (sample standard deviation)

# Multivariate data set

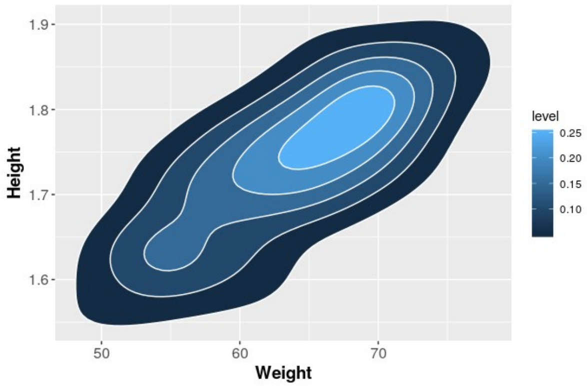


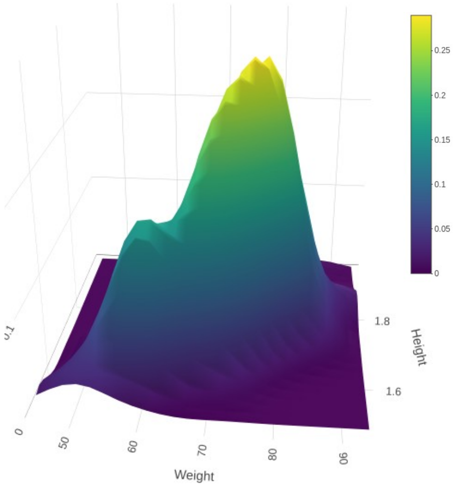

- Two variables

| Participant | Weight (kg) | Height (m) |
|---|---|---|
| S1 | 64 | 1.71 |
| S2 | 80 | 1.82 |
| S3 | 55 | 1.65 |
| S4 | 84 | 1.84 |
| ... | ... | ... |

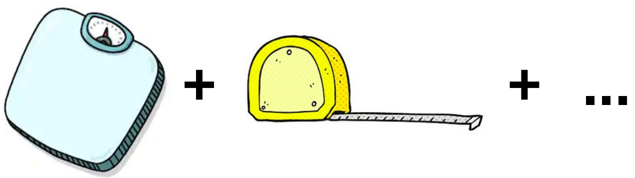



- We can still draw a density plot!



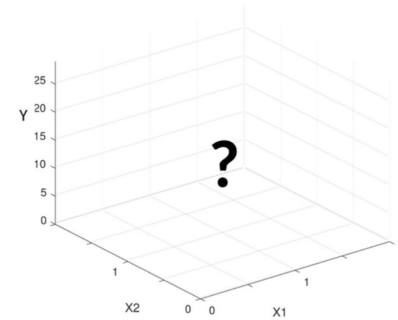
# Multivariate data set



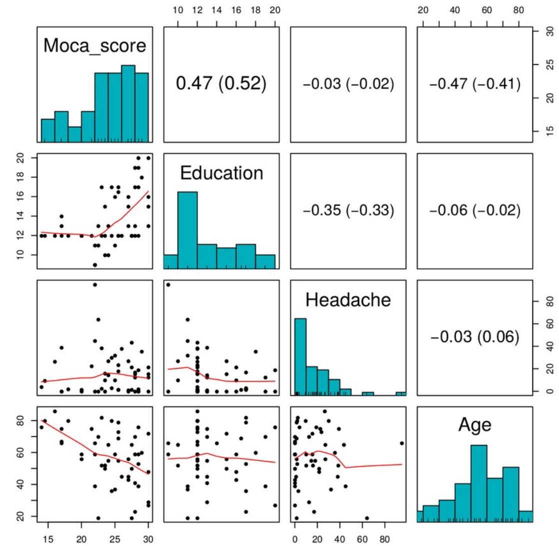

- More than two variables

| Participant | Weight (kg) | Height (m) | ... |
|---|---|---|---|
| S1 | 64 | 1.71 | ... |
| S2 | 80 | 1.82 | ... |
| S3 | 55 | 1.65 | ... |
| S4 | 84 | 1.84 | ... |
| ... | ... | ... | ... |

- Data cannot be visualized anymore...

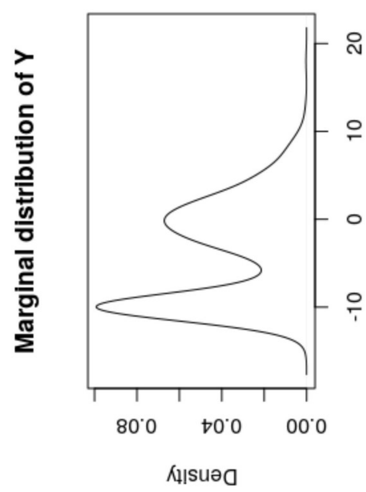


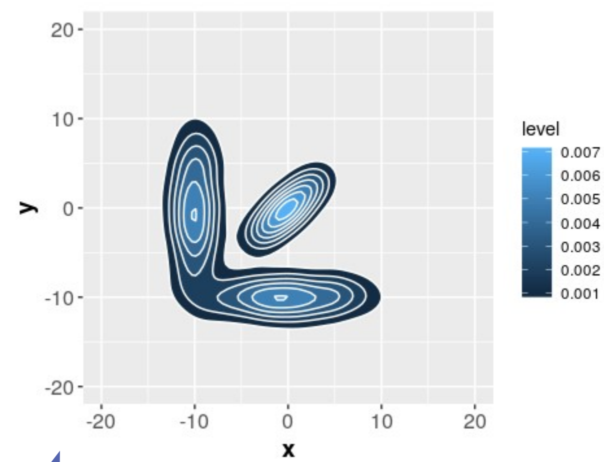

- **Pairs-plot** can help to get an overview of data:

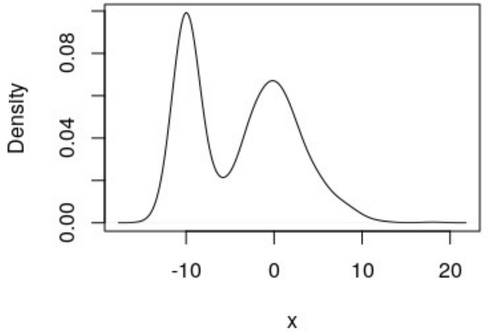


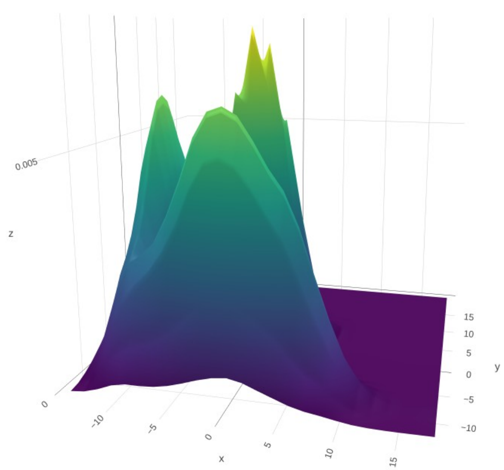
# Multivariate data – descriptive statistics

- Does a multivariate distribution have a **mode**?
  - Yes, the mode is the **most probable realization** of the multidimensional distribution
- The multidimensional mode is **not necessarily composed** of the marginal distributions' modes!



# Multivariate data – descriptive statistics

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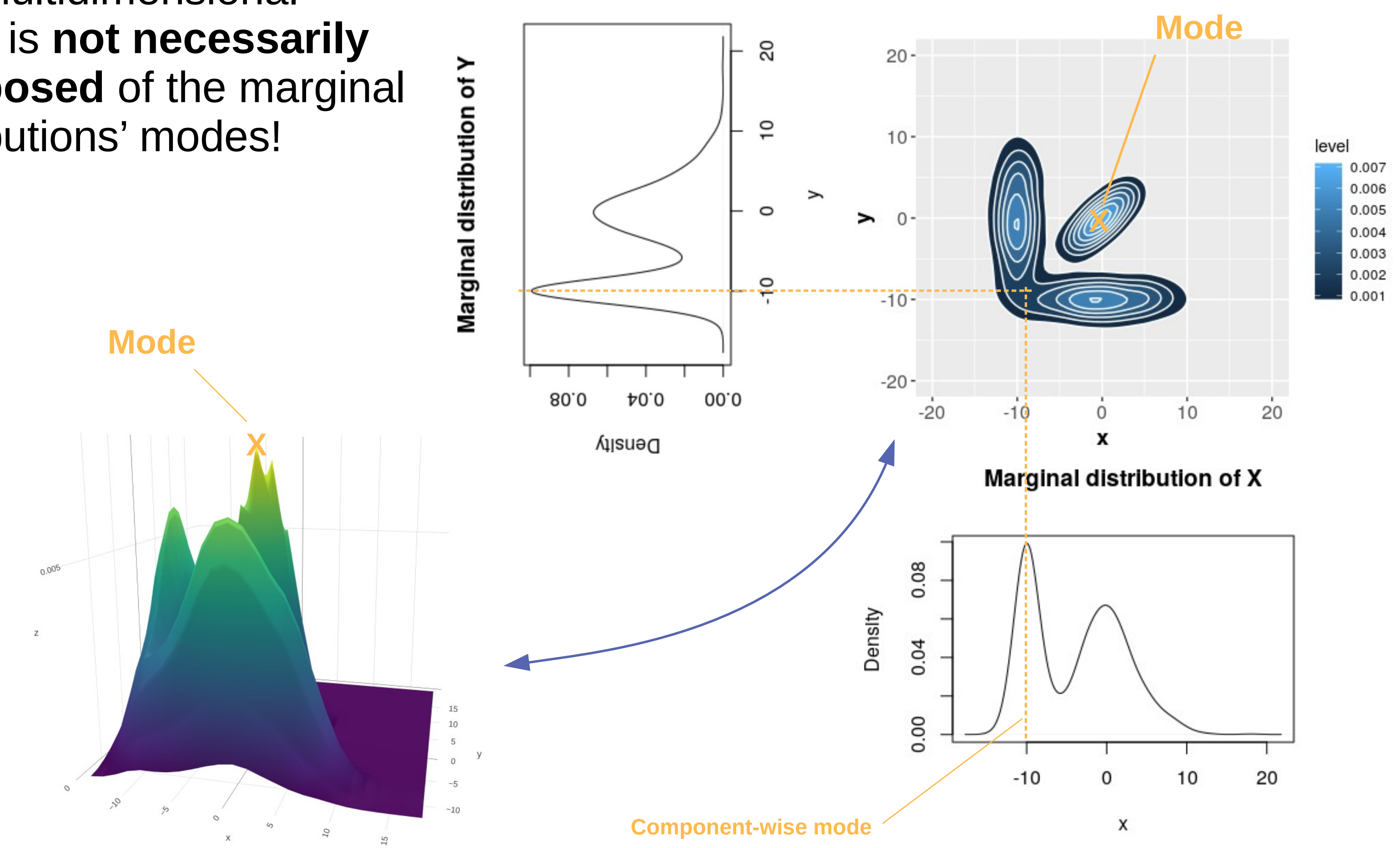
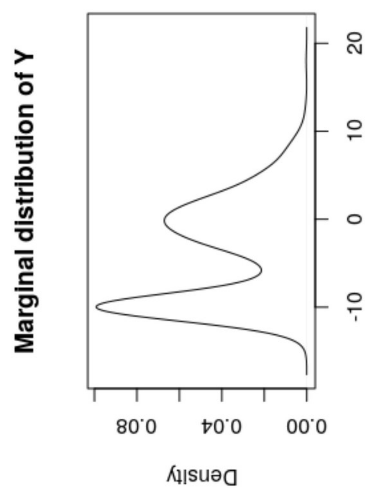
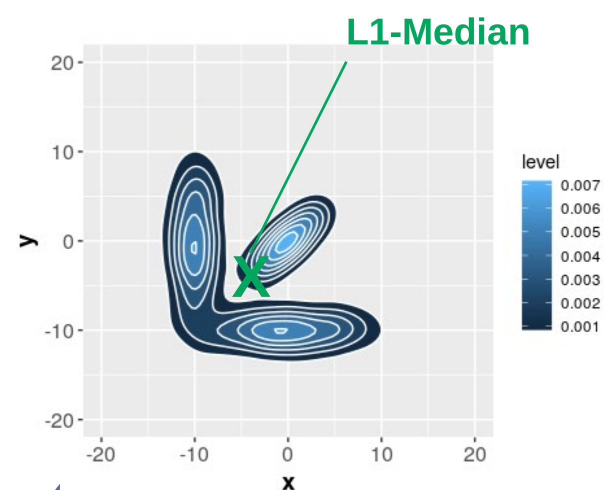
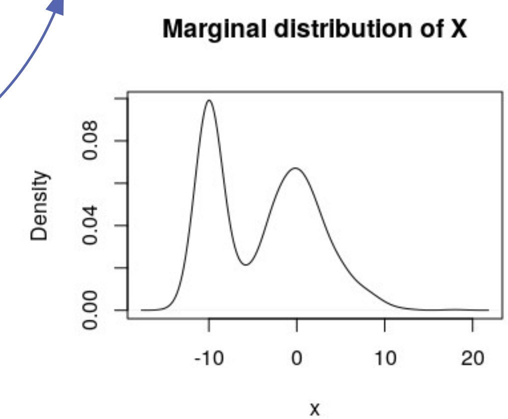


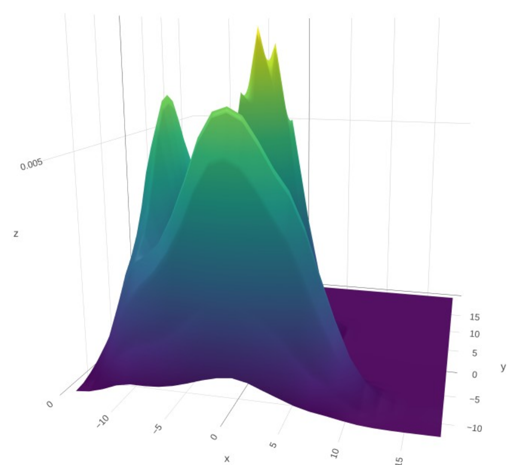
# Multivariate data – descriptive statistics

- Does a multivariate distribution have a **median**?
  - A universally accepted definition of a multivariate median does not exist!
- The “**L1-median**” is the point with a minimal sum of absolute distances to all other points.
- The L1-median does not have to be composed of the component-wise medians!



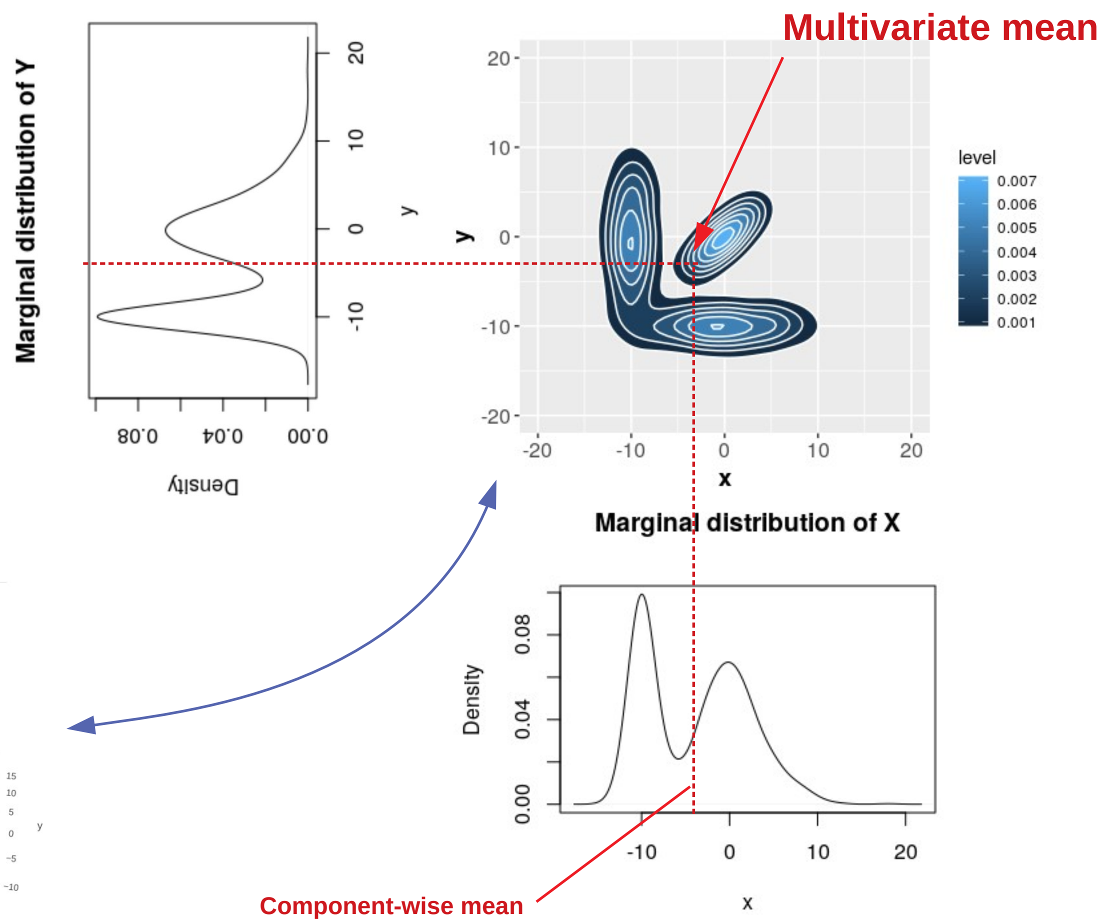



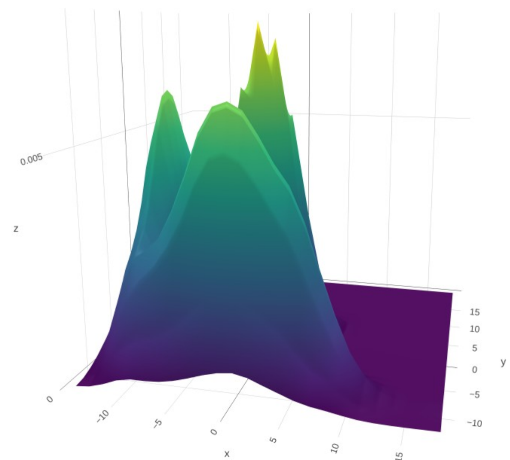



# Multivariate data – descriptive statistics

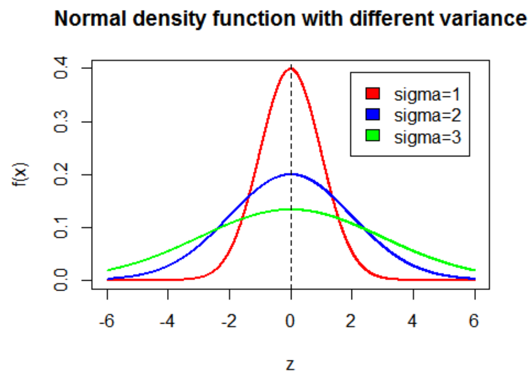
- Does a multivariate distribution have a **mean**?
  - The multivariate mean is the “balance point” of the distribution
- The multivariate mean **is composed** of the marginal distributions’ mean values!



# Variance of multivariate distribution

- Variance is a measure of the amount of “spread” in a univariate distribution




$$s=\sqrt{\frac{\sum(x_i-\bar{x})^2}{n-1}}$$ (sample standard deviation)

The variance is the squared standard deviation:

Var = $s^2$

- In the case of multivariate distributions the variance is represented in a **variance-covariance** matrix

$$\mathbf{S}_{\text{pxp}}=\begin{array}{c|c} & \begin{array}{cccc} X_1 & X_2 & & X_p \end{array} \\ \begin{array}{c} X_1 \\ X_2 \\ \\ X_p \end{array} & \begin{pmatrix} s_1^2 & s_{12} & \cdots & s_{1p} \\ s_{21} & s_2^2 & \cdots & s_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ s_{p1} & s_{p2} & \cdots & s_p^2 \end{pmatrix} \end{array}$$

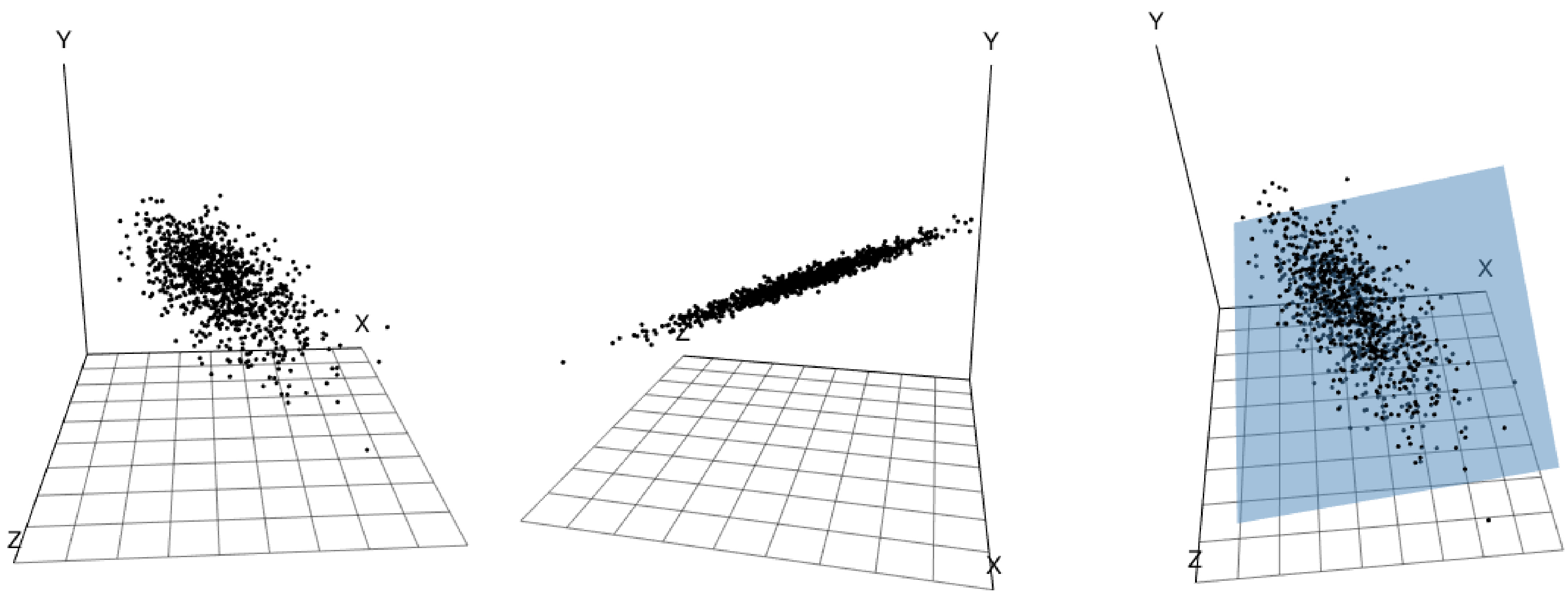
The diagonal elements hold the variances of variables

The off-diagonal elements hold the covariance between the respective variables

$$Cov(x,y)=\frac{\sum(x_i-\bar{x})^2(y_i-\bar{y})^2}{n-1}$$ (sample covariance)

# Dimensionality reduction

- Is the high number of dimensions really necessary to represent the data?
- Example: The data below is almost lying on a plane
  - The data could also be represented in a two-dimensional coordinate system, without losing a lot of information



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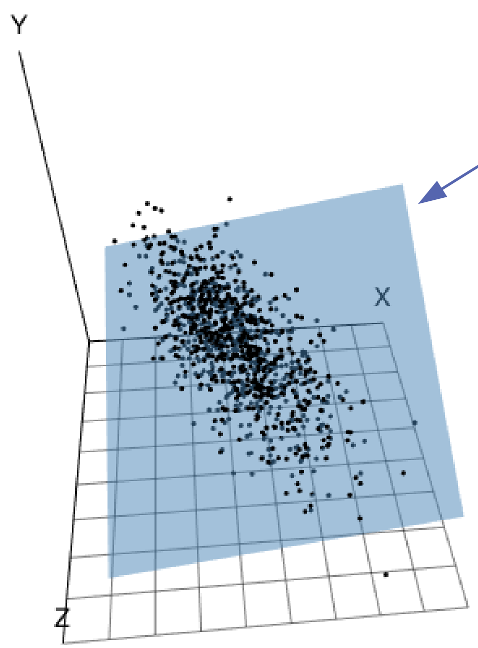
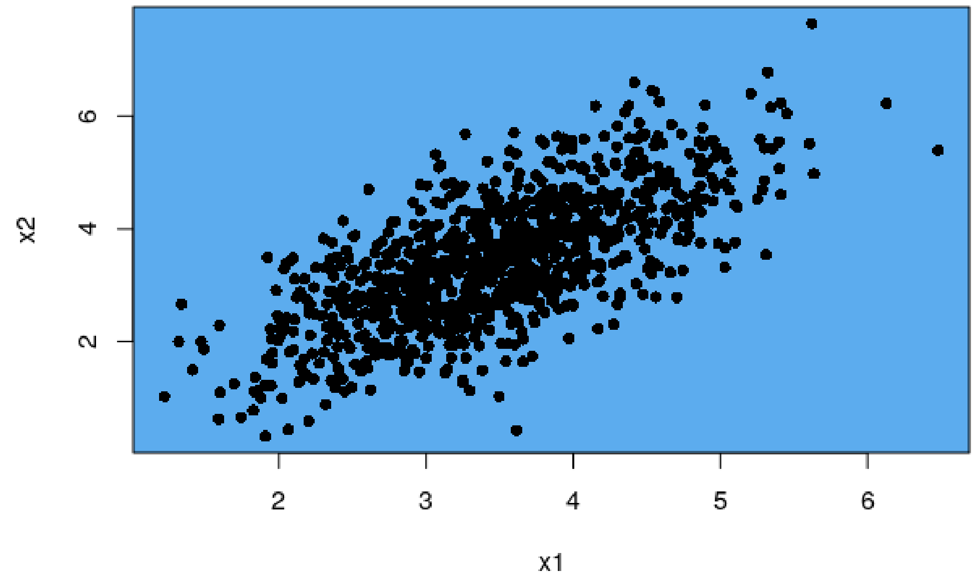


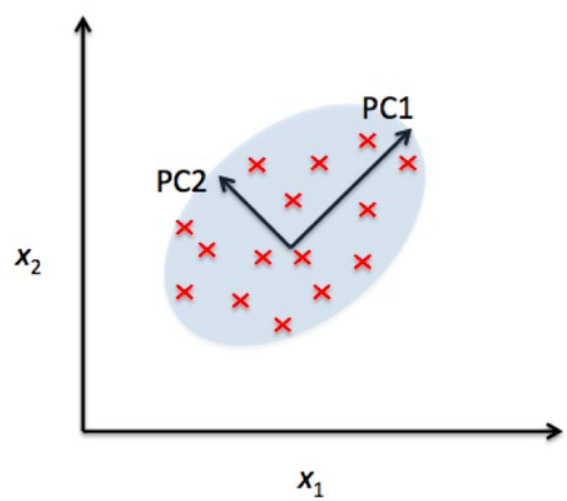

Went from **three** dimensions down to a representation in **two** dimensions by taking the blue plane as the new coordinate system



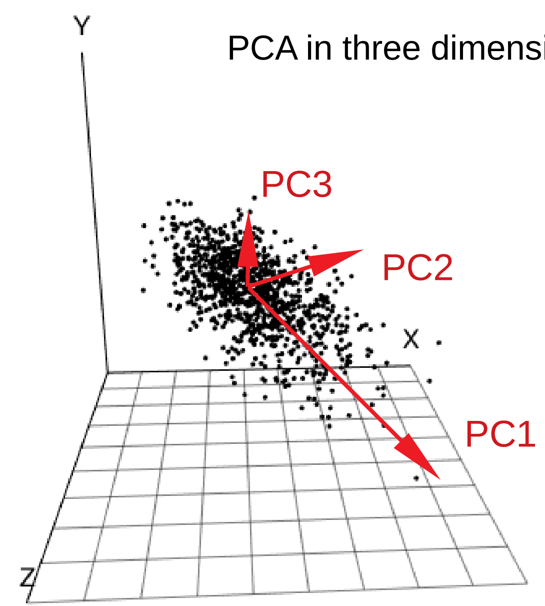
# Principal Component Analysis

- **PCA** (**Principal Component Analysis**) is a common method used for dimensionality reduction
- The idea behind PCA is a rotation of the coordinate system (new axes are principal-component 1, principal-compoinent2, …)
  - **Principal-component 1** is the direction in which the data shows the **highest variance**
  - **Principal-component 2** lies **orthogonal** to PC1 and is the direction of the second-highest variance
  - ...

PCA in two dimensions

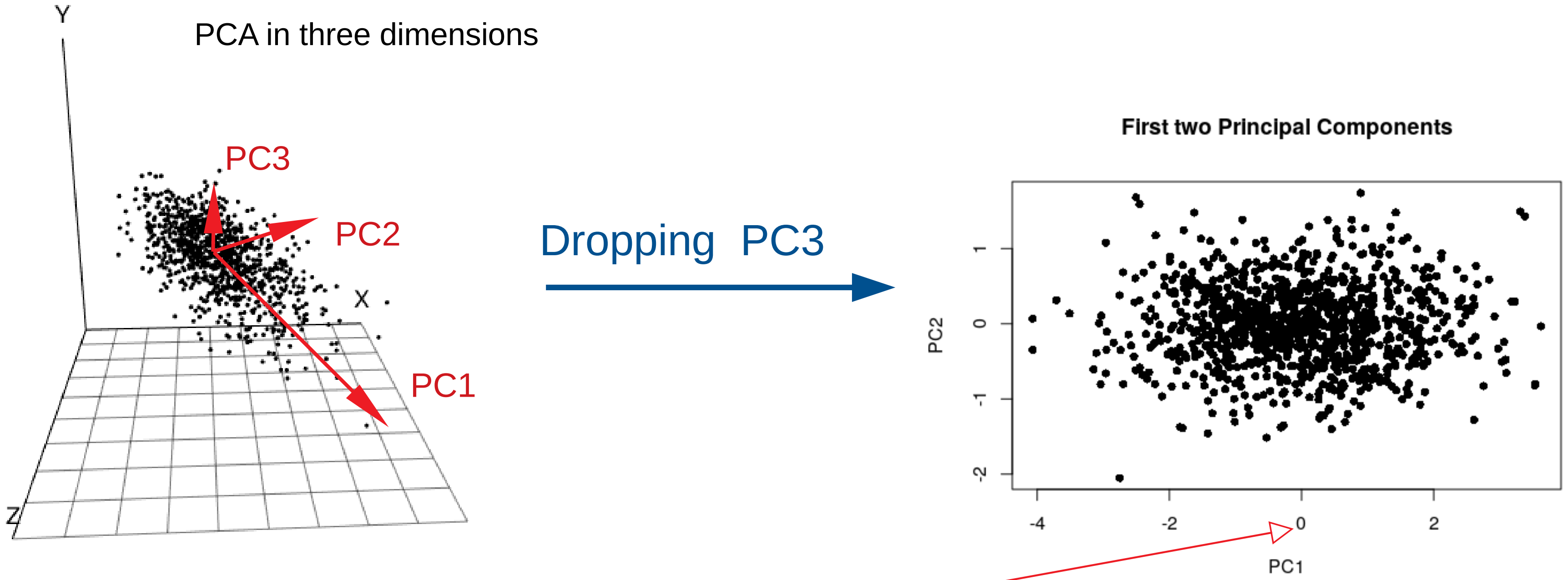



PCA in three dimensions



# Principal Component Analysis

- In practice, the goal is often to visualize the high-dimensional data in a 2D-plot, by dropping all principal components except the first two:




- The data is centered (subtracting the mean value from each variable, respectively) when PCA is applied
  - Often the data is also scaled (see later slides)

# How do we find the PCs?

- After the data has been centered, PCA is just a rotation of the coordinate system (no information is lost)
  - PCA is always possible, one just has to find the right rotation matrix
- It can be shown with linear algebra, that finding the rotation matrix is easier than expected
- The rotation matrix is formed by the **eigen-vectors** of the **variance-covariance-matrix** of the centered data
  - In the case of scaled data, the principal components are the eigen-vectors of the correlation matrix

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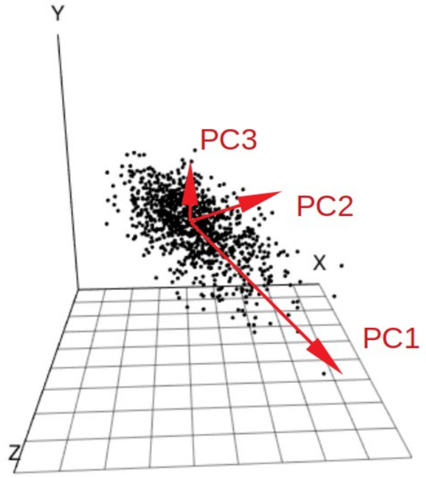
# PCA in R

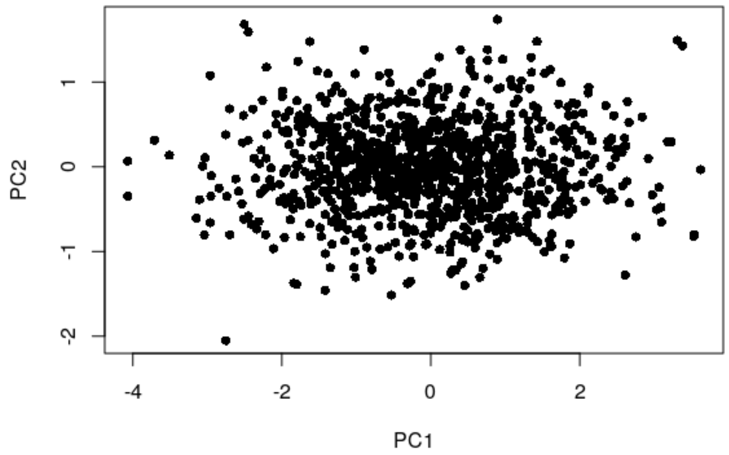
- PCA can be performed in R using the **prcomp()** function

```
> pc <- prcomp(x = myData)  # perform PCA
> summary(pc)
Importance of components:
                          PC1    PC2     PC3
Standard deviation     1.270 0.5430 0.08999
Proportion of Variance 0.842 0.1538 0.00423
Cumulative Proportion  0.842 0.9958 1.00000
```




- Plot the first two PCs:

```
> plot(PC2~PC1, data=pc$x)
```



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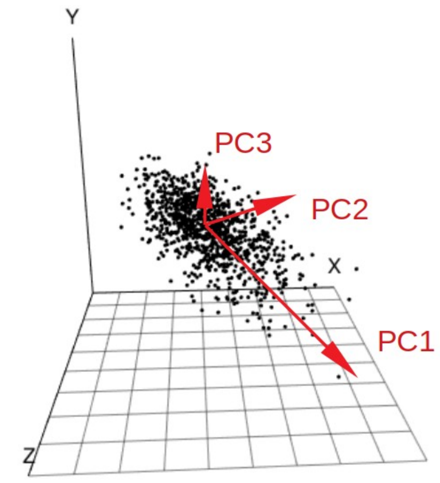
# PCA in R

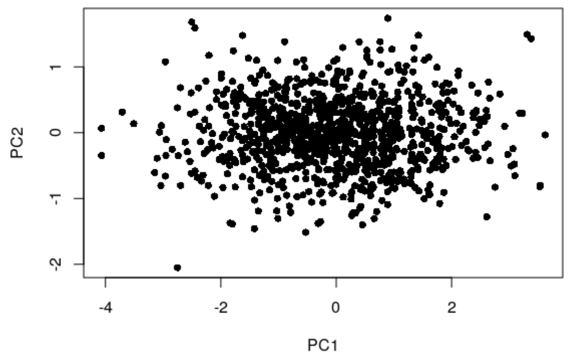
- PCA can be performed in R using the **prcomp()** function

```
> pc <- prcomp(x = myData)  # perform PCA
> pc
Standard deviations (1, .., p=3):
[1] 1.27035807 0.54295340 0.08998992

Rotation (n x k) = (3 x 3):
          PC1        PC2        PC3
x  0.4918003  0.8525767  0.1767639
y -0.2408321  0.3282877 -0.9133603
z  0.8367391 -0.4066205 -0.3667798
```

shows the contribution of the individual variables to the PCs
(also referred to as **variable loadings**)



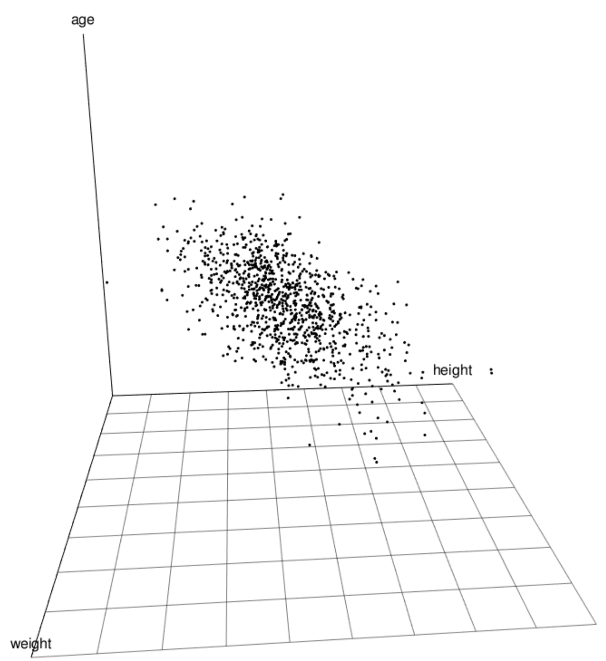



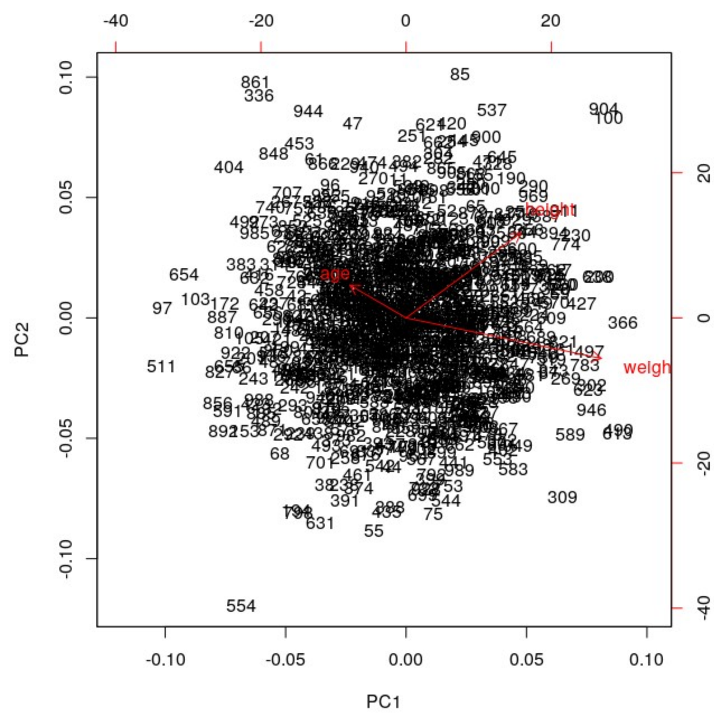

- The first principal component is composed in the following way:

PC1 = 0.4918003***x** – 0.2408321***y** + 0.8367391***z**

# Biplot – projection of variables

- In Biplots the original variables are projected into the PC-coordinate system
  - Gives an impression of the contribution of each variable to the PCs



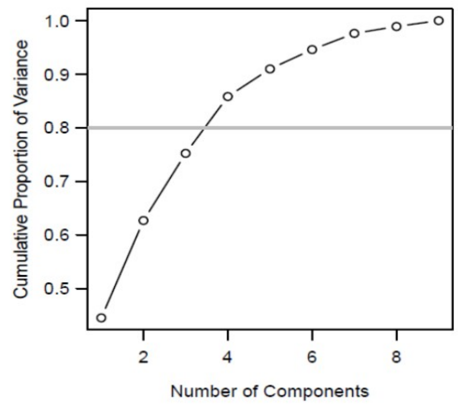




- In R:

```
> pc <- prcomp(x = myData)  # perform PCA
> biplot(pc)
```

# How many PCs are needed?

- Take a look at the explained variance by the PCs
- Rule of thumb is that **~80% of total variance** should be explained by the first k PCs

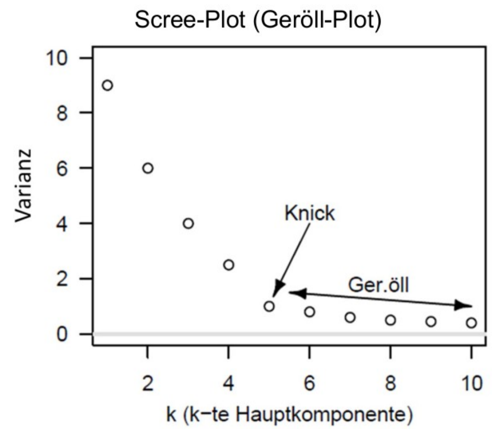



proportion of variance explained by the first k principle components:

$$P_k = \frac{\sum_{j=1}^{k} \mathrm{var}(Y_j)}{V_{total}} \in [0,1]$$

→ Following this rule, we need the **first four PCs** to explain data

- Other method: Check for a “bend” in the Scree-Plot (Geröll-Plot)




```
# In R:
> screeplot(pca_object, npcs=10, type=”l”)
```

→ In this case, we need the **first four PCs**, afterwards not much more information is won

# When to scale the data?

- Often the data is scaled before performing the PCA
- Scaling means that the values of each variable are divided by the variable's standard deviation
  - Now, every variable has unit-variance (variance = 1)
  - **Scaling does affect the results of the PCA**! (e.g. variable measured in ms vs variable in hours, see covariance-table below)
- In R scaling can be set in the options of the **prcomp()** command
  - Default is not to scale: prcomp(mydata, scale.=FALSE)
- Scaling is generally **advisable** when the variables have **different scales** (e.g. cm, m, kg, …)
- Scaling is **not advised** when the variables have the **same scale** and are comparable with respect to their variability

→ Example: "Assault" will have a large contribution to PC1 because of its large variance (see covariance matrix)

| | Murder | Assault | UrbanPop | Rape |
|---|---|---|---|---|
| Murder | 18.970465 | 291.0624 | 4.386204 | 22.99141 |
| Assault | 291.062367 | 6945.1657 | 312.275102 | 519.26906 |
| UrbanPop | 4.386204 | 312.2751 | 209.518776 | 55.76808 |
| Rape | 22.991412 | 519.2691 | 55.768082 | 87.72916 |