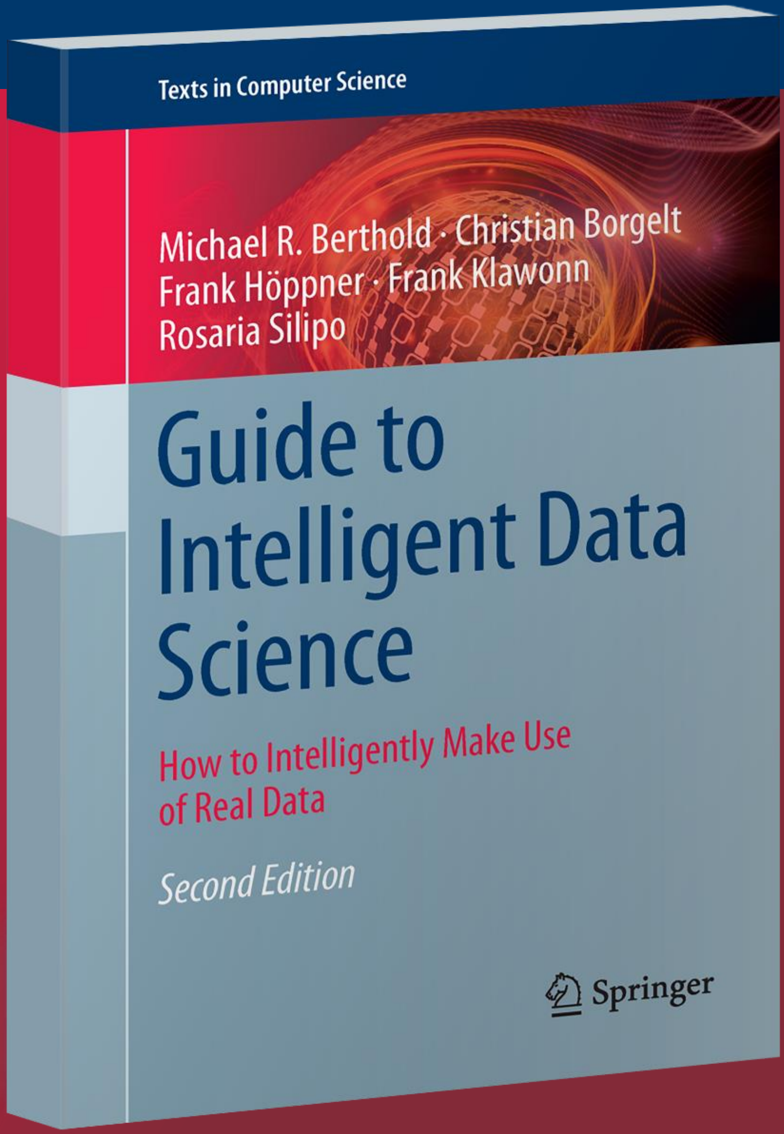
Data Visualization



„There is no excuse for failing to plot and look“

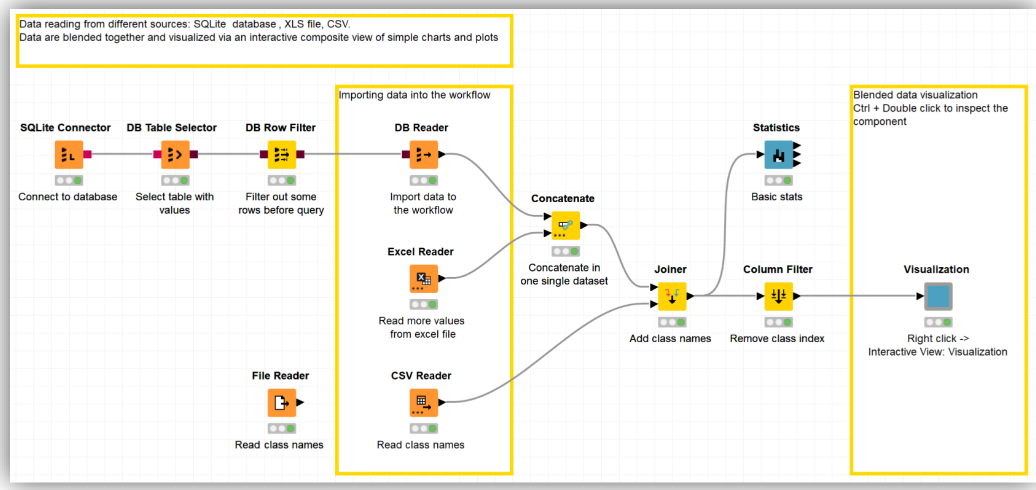
What is the best way of plotting a dataset?

**This lesson refers to chapter 4 of the GIDS book*

- Methods for One and Two Attributes
  - Barchart and Histogram
  - Boxplot
  - Scatter plot and density plot

- Methods for Higher-dimensional Data
  - Principal Component Analysis (PCA)
  - Multidimensional Scaling (MDS)
  - t-distributed Stochastic Neighbor Embedding (t-SNE)
  - Parallel Coordinates
  - Radar and Star Plots
  - Sunburst Chart
  - Correlation Analysis

- Datasets used : adult dataset and outliers dataset
- Example Workflows:
  - „Simple Visualizations“ https://kni.me/w/dwugN1qYM2OOjzO4
    - Read from CSV file, Excel file and SQLite.
    - bar chart and histogram
    - parallel coordinates
    - box plot
    - scatter plot
    - table view.



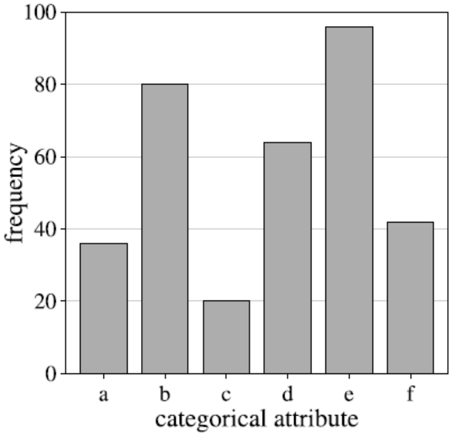
Statistical Descriptors

Statistical measures can be used to describe a dataset:

- Range
- Min/max values
- Mean $\mu = \frac{1}{n}\sum_{i=1}^{n} x_i$
- Variance $\sigma^2 = \frac{1}{n-1}\sum_{i=1}^{n}(x_i - \mu)^2$
- Standard deviation $\sigma = \sqrt{\frac{1}{n-1}\sum_{i=1}^{n}(x_i - \mu)^2}$
- Median (The middle number; found by ordering all data points and picking out the one in the middle - or if there are two middle numbers, taking the mean of those two numbers)
- Mode (Most frequently occurring value)
- Percentiles (Quartiles)
- Number of missing values
- ...

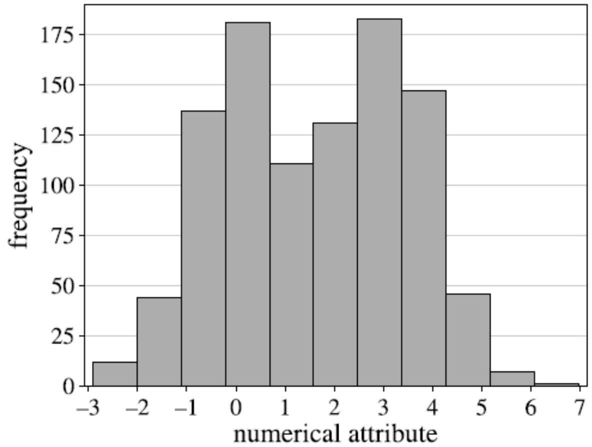
Visualization Methods for One Attribute

Bar chart

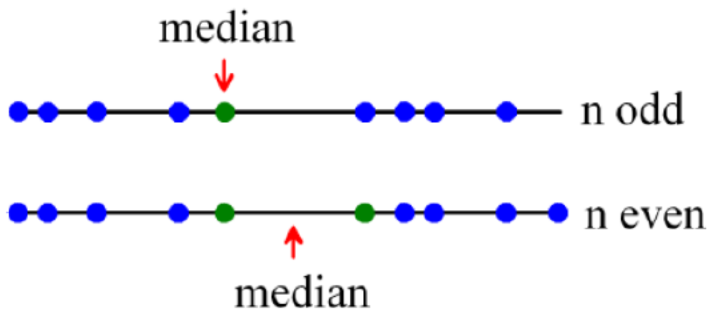


– A bar chart is a simple way to depict the frequencies of the values of a categorical attribute.

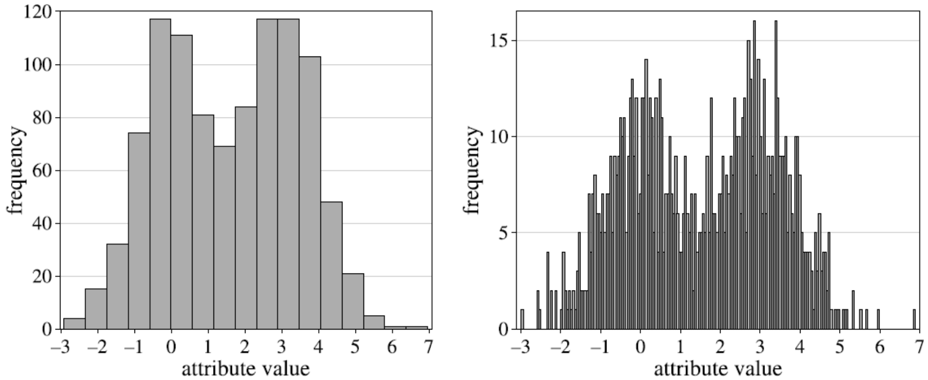
Histogram



- A histogram shows the frequency distribution for a numerical attribute.
- The range of the numerical attribute is discretized into a fixed number of intervals (bins), usually of equal length.
- For each interval, the (absolute) frequency of values falling into it is indicated by the height of a bar.



- **Median:** The value in the middle (for values sorted in increasing order)
- **q%-quantile** (0 < q < 100): The value for which q% of the values are smaller and 100-q% are larger. The median is the 50%-quantile
- **Quartiles**: 25%-quantile (1st quartile), median (2nd quantile), 75%-quantile (3rd quartile)
- **Interquartile range (IQR):** 3rd quartile – 1st quartile



- **Best choice for number k of bins in the histogram?**
- Sturge‘s Rule $k = \lceil log_2(n) + 1 \rceil$
- Through fixed bin length h

$$k = \left\lceil \frac{max_i\{x_i\} - min_i\{x_i\}}{h} \right\rceil \text{ with } h = \frac{3.5 \cdot s}{n^{\frac{1}{3}}} \quad \text{or} \quad h = \frac{2 \cdot IQR\,(x)}{n^{\frac{1}{3}}}$$

Where s is the standard deviation of input feature x, x_i its value in the i-th sample, and n the number of samples in the dataset.

- **Skewness** is the 3rd standardized moment of X, that is:

$$\tilde{\mu}_3 = E\left[\left(\frac{X-\mu}{\sigma}\right)^3\right] = \frac{E[(X-\mu)^3]}{E[(X-\mu)^3]} = \frac{\mu_3}{\sigma^3}$$

- Skewness measures the asymmetry of the probability distribution of X

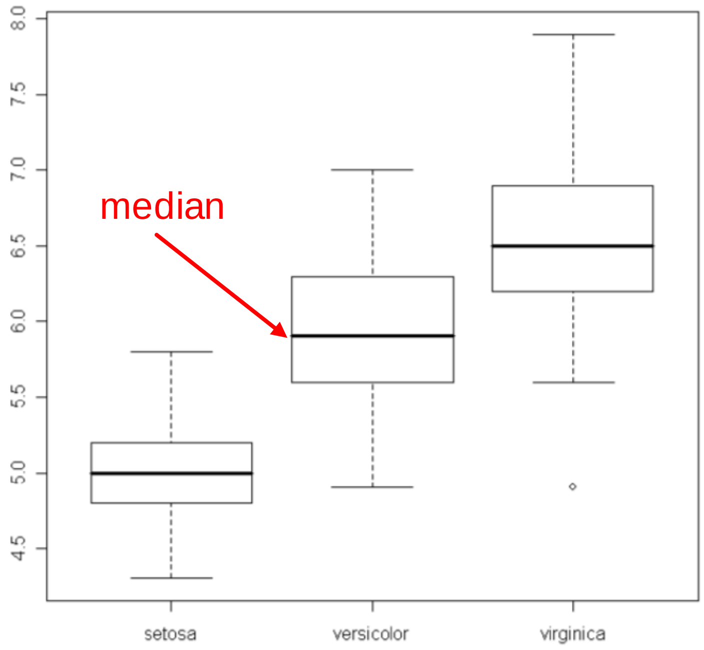
- **Kurtosis** is the 4th standardized moment of X, that is:

$$Kurt[X] = E\left[\left(\frac{X-\mu}{\sigma}\right)^4\right] = \frac{E[(X-\mu)^4]}{(E[(X-\mu)^2])^2} = \frac{\mu_4}{\sigma^4}$$

- Kurtosis measures the devaition from the peak in a Gaussian distribution: it measures the dispersion due to outliers
- Kurtosis of any univariate normal distribution is 3

Boxplots

- Boxplots are a very compact way to visualize and summarize the main characteristics of a numeric attribute, through the ***median***, the IQR, and possible outliers



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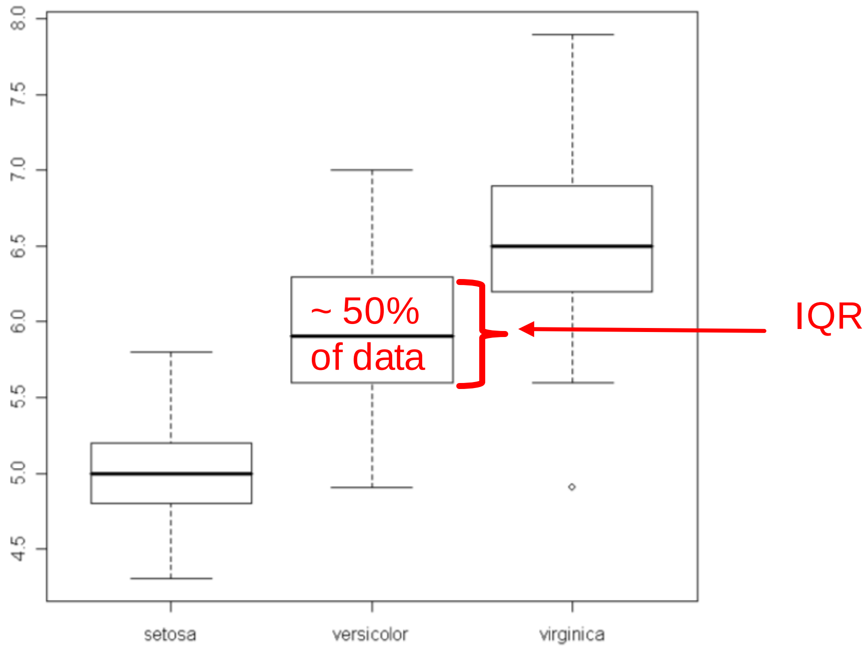

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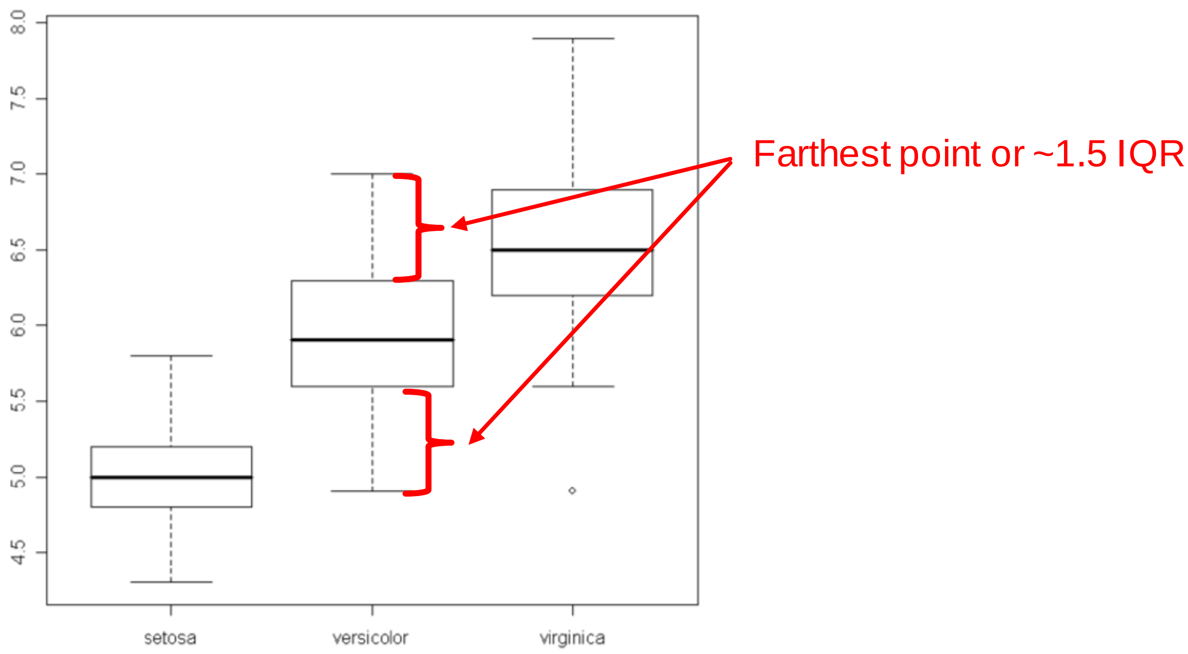

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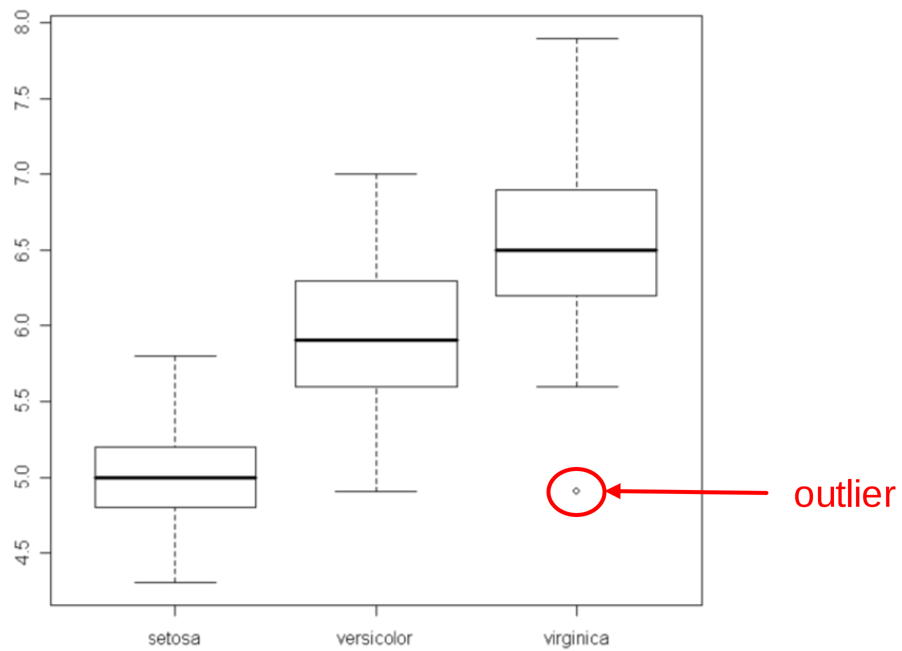
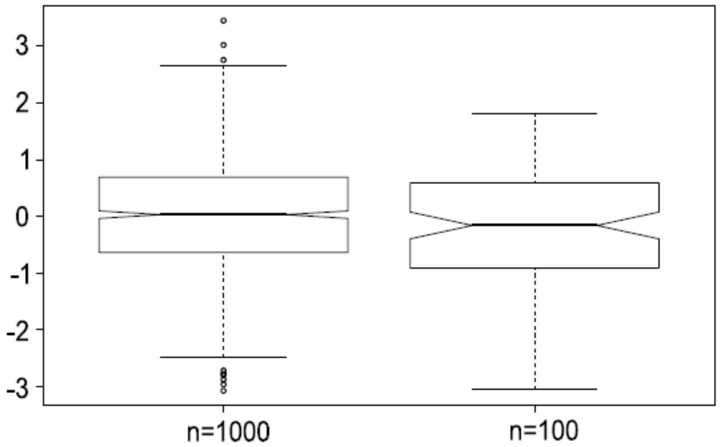


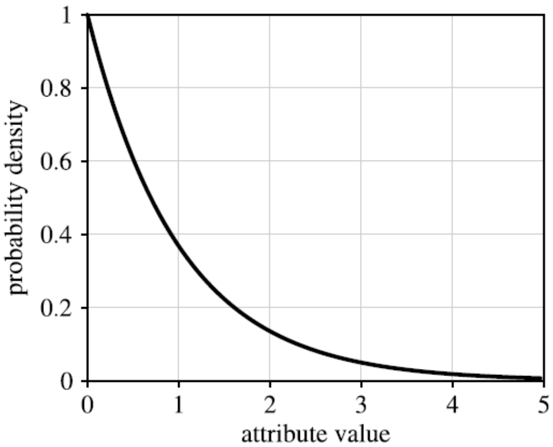
- The same distribution can result in different boxplots
- This depends on the sample size n
- Two samples from normal distribution with different size n
- For the small sample:
  - Whiskers have different length, even if it is the same symmetric distribution
  - No outliers



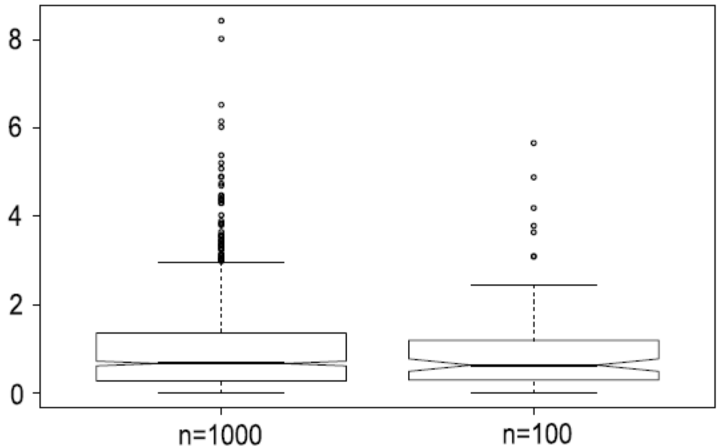
Boxplots from different samples from a standard normal distribution

Boxplot of asymmetric distribution

– Boxplots of different samples from exponential distribution with $\lambda = 1$



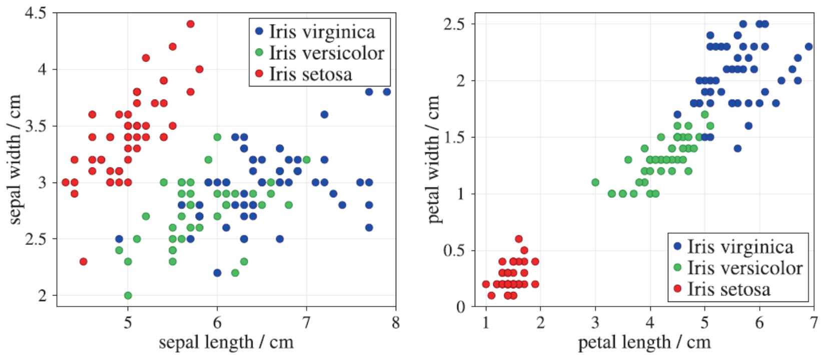
Exponential distribution with $\lambda = 1$



Boxplots from different samples from exponential distribution with $\lambda = 1$

Visualization Methods for Two Attributes

Scatter Plot

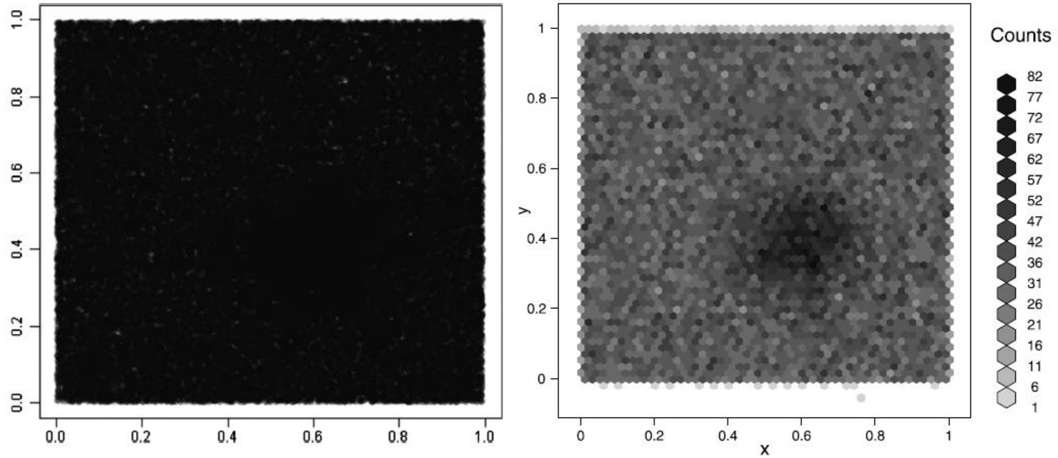


Petal length and width provide better class separation than sepal length and width

Scatter plots of the Iris data set for sepal length vs. sepal width (left) and for petal length vs. petal width (right). All quantities are measured in centimetres

- In scatter plots two attributes are plotted against each other
- Can be enriched with additional features (color, shape, size)
- Suitable for small number of points; not suitable for large datasets
- Points can hide each other -> add **Jitter** (a small random value to each point)

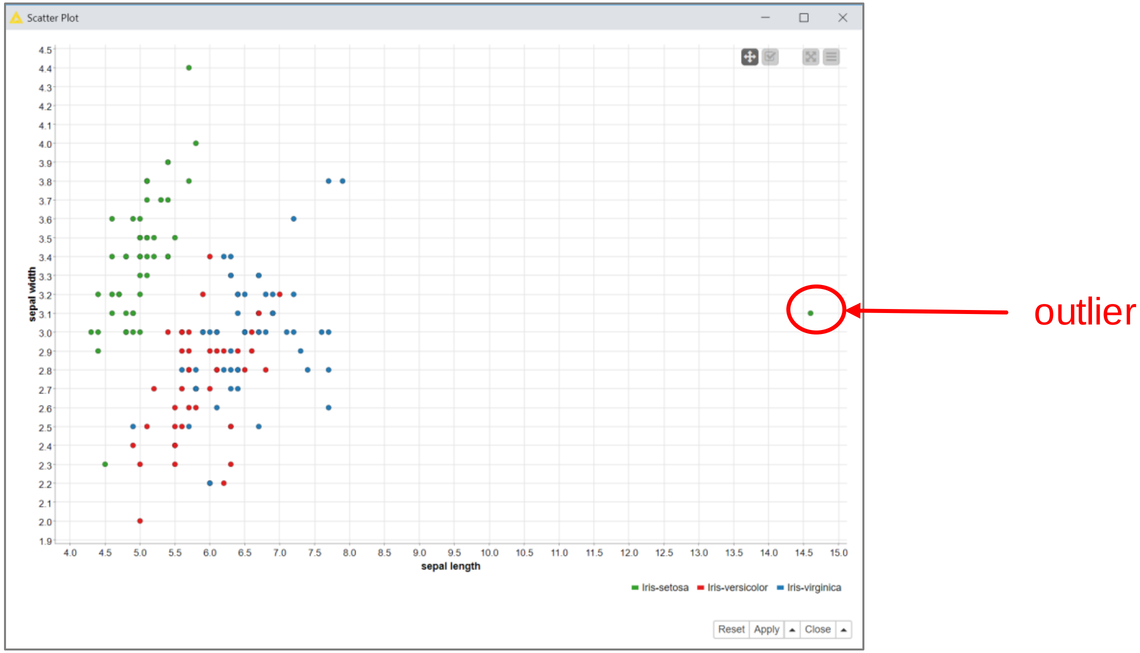
Scatter Plot



Density plot (left) and a plot based on hexagonal binning (right) for a dataset with n = 100,000 instances

- Scatter plot is not suitable for large datasets
- Alternatives:
  - Density plot for example using semi-transparent points: the more points in the same place the less transparent
  - Binning points into rectangles or hexagons and heat scale color

– Scatter plots can be used to detect outliers

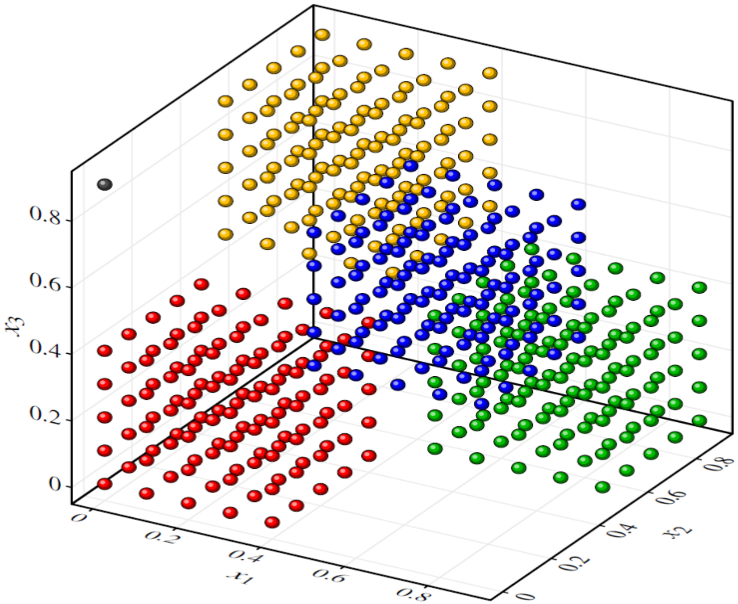


- Visualization can be used as a test

- **Good News**
  - Visualization reveals patterns or exceptions => there is something in the dataset
- **Bad News**
  - Visualization does not indicate anything specific => there might still be something in the dataset even if we do not see it
  - For example, if we do not see outliers for that combination of features, that does not mean that outliers do not exist in the dataset.

Methods for Higher-Dimensional Data

A display or plot is **by definition two-dimensional**, so that only max. two axes (attributes) can be incorporated.
3D techniques can be used to incorporate three axes (attributes).

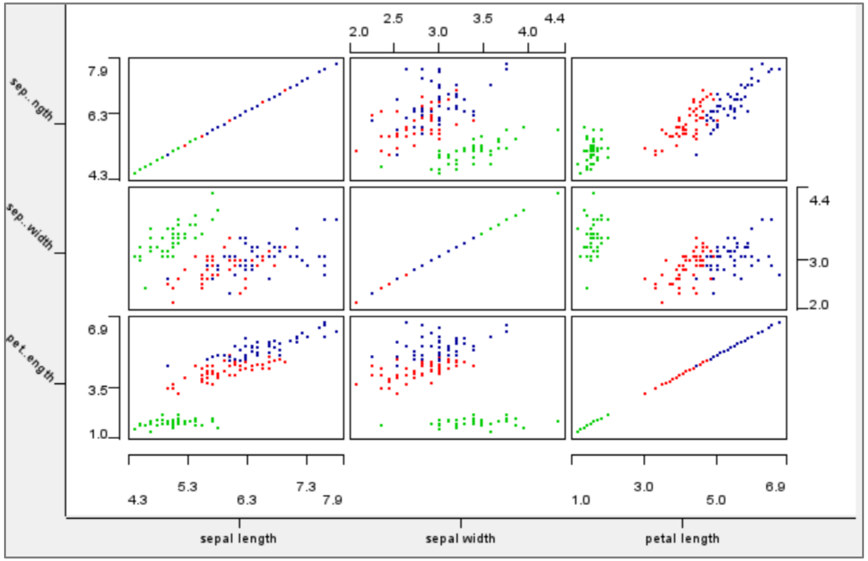


3D scatter plot

Example

- A data set distributed over a cube in a **chessboard-like pattern**.
- The colors are only meant to make the different cubes more easily discernible. They do not indicate classes.
- Note the outlier in the upper left corner

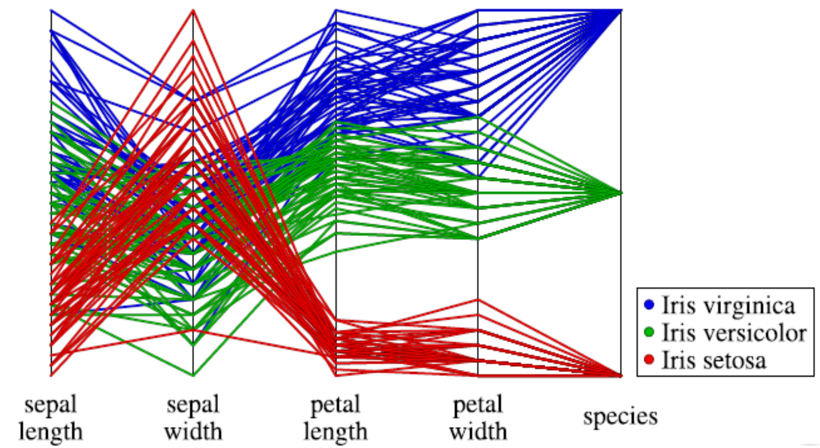
- A matrix of scatter plots $m \times m$ where m is the number of attributes (data dimensionality)
- For m attributes there are $\binom{m}{2} = m(m-1)$ possible scatter plots
- e.g. For 50 attributes there are 2450 scatter plots!



Scatter matrix

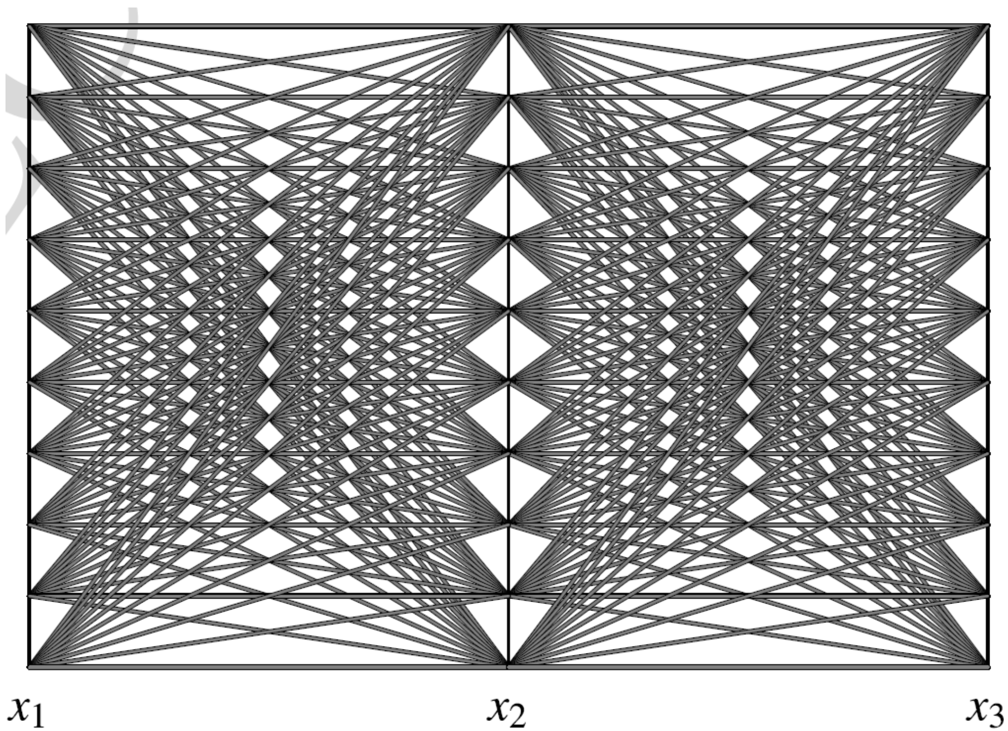
Parallel Coordinates Plot

- Parallel coordinates draw the coordinate axes for each attribute parallel to each other, so that there is no limitation for the number of axes to be displayed.
- For each data object, a polyline is drawn connecting the values of the attributes on the corresponding axes.
- Maintains the original attributes
- Limited number of entries
- How do we spot correlation between features?

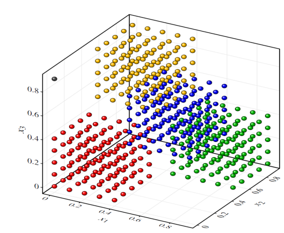


Parallel coordinates plot for the Iris data set

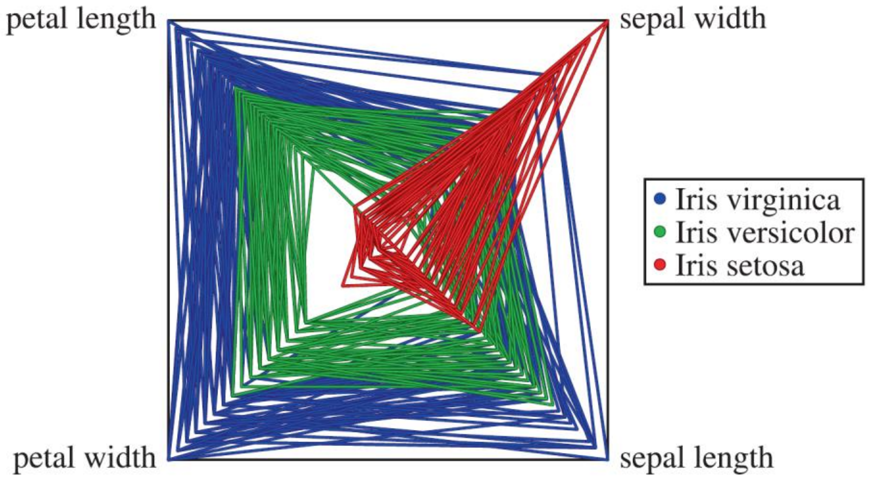
Parallel Coordinates Plot: „Cube Data“



Parallel coordinates plot for the Cube data

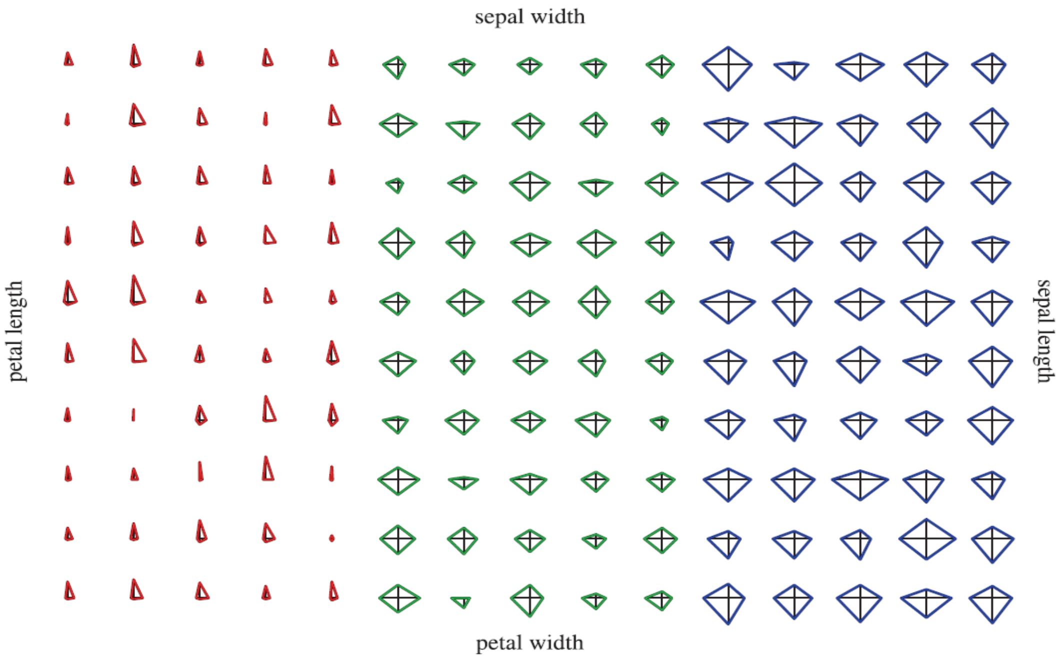


- Similar idea of the Parallel Coordinates plot
- Axes are drawn in a star-like fashion intersecting in one point
- Also called spider plots
- Suitable for small datasets



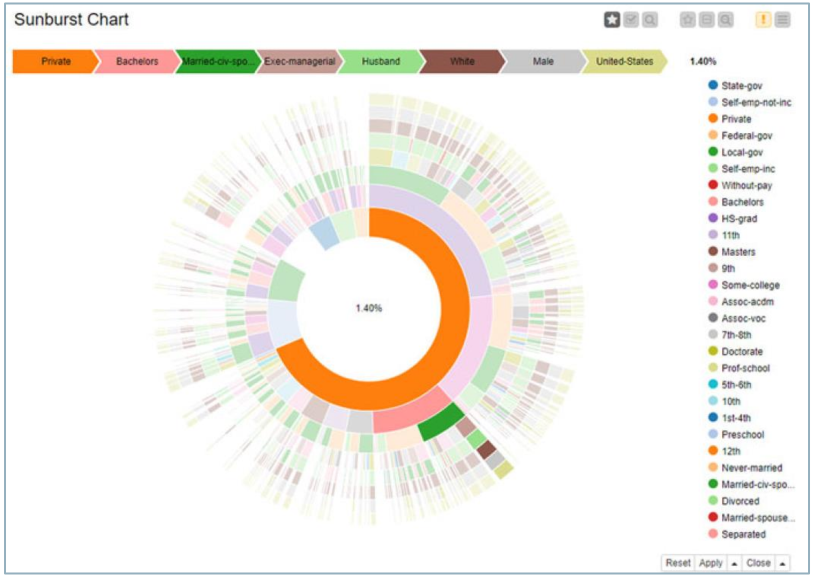
Radar plot for the Iris data set

- In a star plot each object is drawn separately
- In a radar plot fashion



Star plot for the Iris data set

Sunburst Chart



– Display multidimensional hierarchical nominal data in a radial layout
– One section ⇔ one attribute
– Root attribute in the center, external sections are attributes located deeper in the hierarchy
– Area of a section represents the accumulated value of all descending sections

How can we transform a higher-dimensional data set to have two or three dimensions?

- Preserve as much of the “structure” of the original data
- Define a measure to evaluate how well the original structure of the high-dimensional dataset is preserved after transformation
- Find the transformation that gives the best value for the given measure

Correlation Analysis

How can we measure the similarity in behavior of two attributes?

- Pearson's correlation coefficient
- Spearman's rank correlation coefficient (Spearman's rho)

- **Pearson's correlation coefficient** is a measure for the **linear relationship** between two **numerical** attributes *X* and *Y* and is defined as:

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

- where $\bar{x}$ and $\bar{y}$ are the (sample) mean values of the attributes *X* and *Y*, respectively, and s_x and s_y are the corresponding (sample) standard deviations
- $-1 \leq r_{xy} \leq 1$
- The larger the absolute value of the Pearson correlation coefficient, the stronger the linear relationship between the two attributes. For $|r_{xy}|$ = 1 the values of *X* and *Y* lie exactly on a line.
- Positive (negative) correlation indicates a linear relationship (a line) with positive (negative) slope.

- **Spearman's rank correlation coefficient (Spearman's rho)** is defined as:

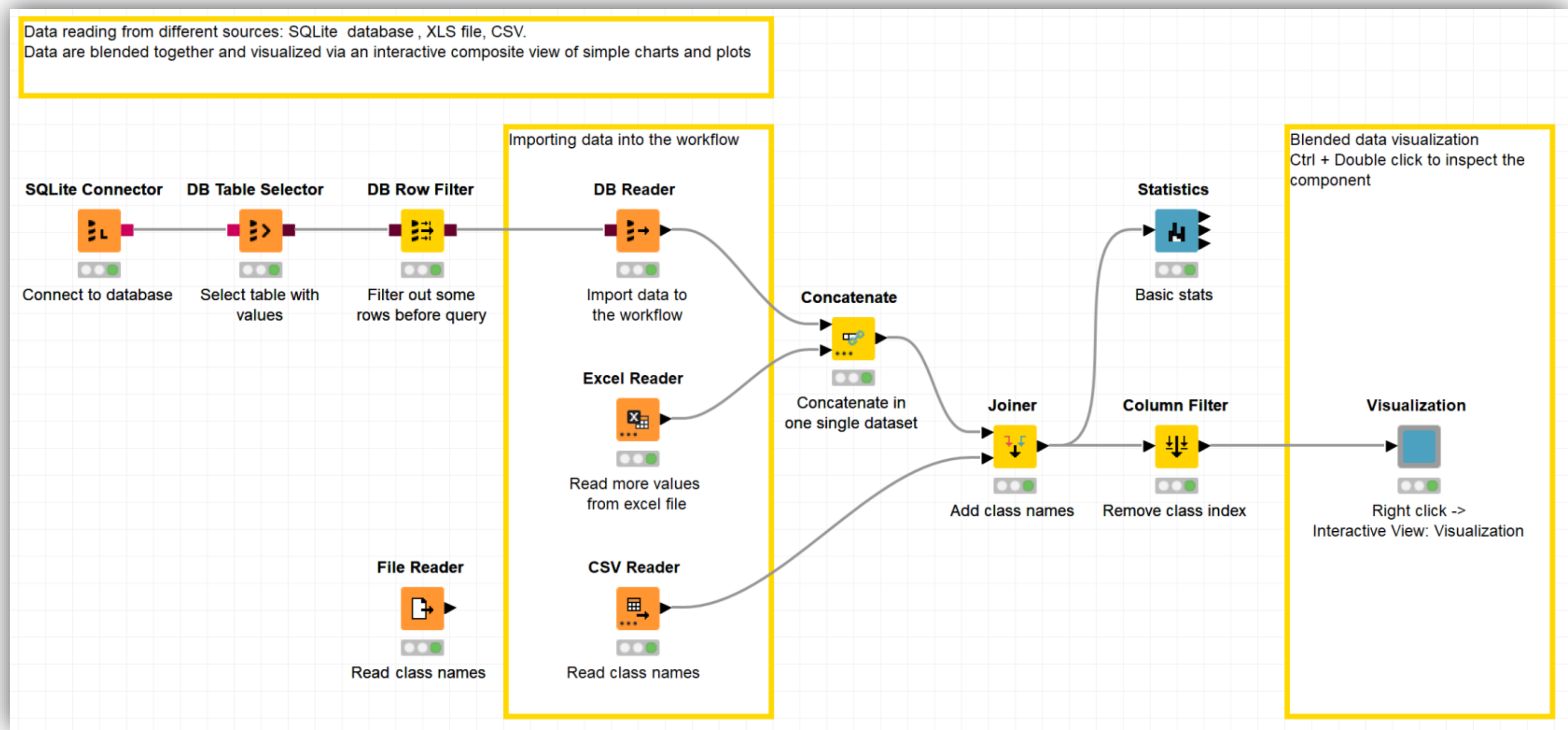
$$\rho = 1 - 6 \frac{\sum_{i=1}^{n}\left(r(x_i) - r(y_i)\right)^2}{n\,(n^2 - 1)}$$

where $r(x_i)$ is the rank of value x_i when we sort the list $(x_1, x_2, \ldots, x_n)$ in increasing order. $r(y_i)$ is defined analogously.

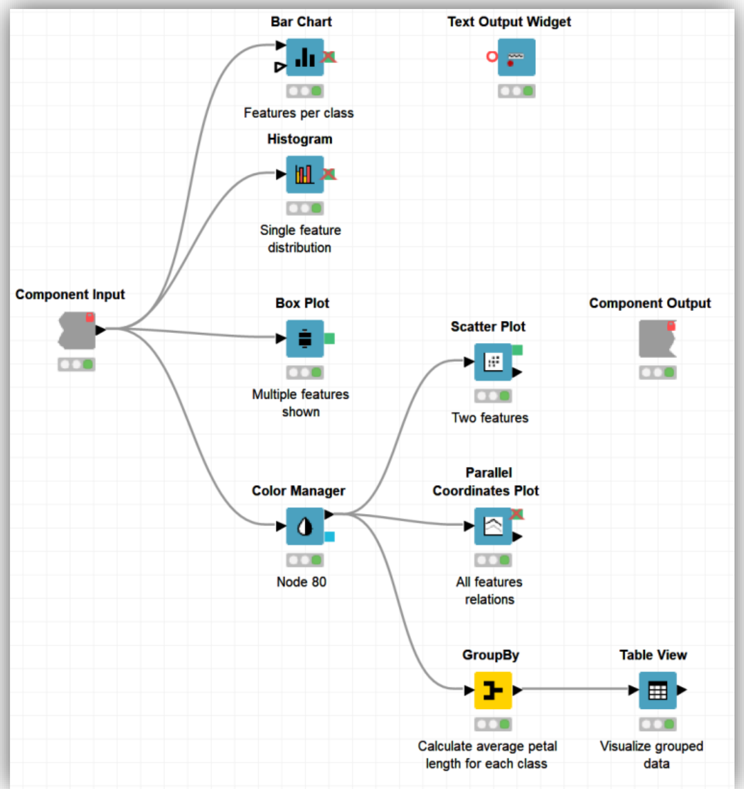
- When the rankings of the *x*- and *y*-values are exactly in the same order, Spearman's rho will yield value 1.
- If they are in reverse order, Spearman's rho will yield value −1.

Practical Examples with KNIME Analytics Platform

– Simple visualization



– Inner workings of the visualization component



– Interactive view

Summary

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Thank you

For any questions please contact: education@knime.com