Introduction to Data Mining

Web Chapter
Exploring Data

by Michael Hahsler

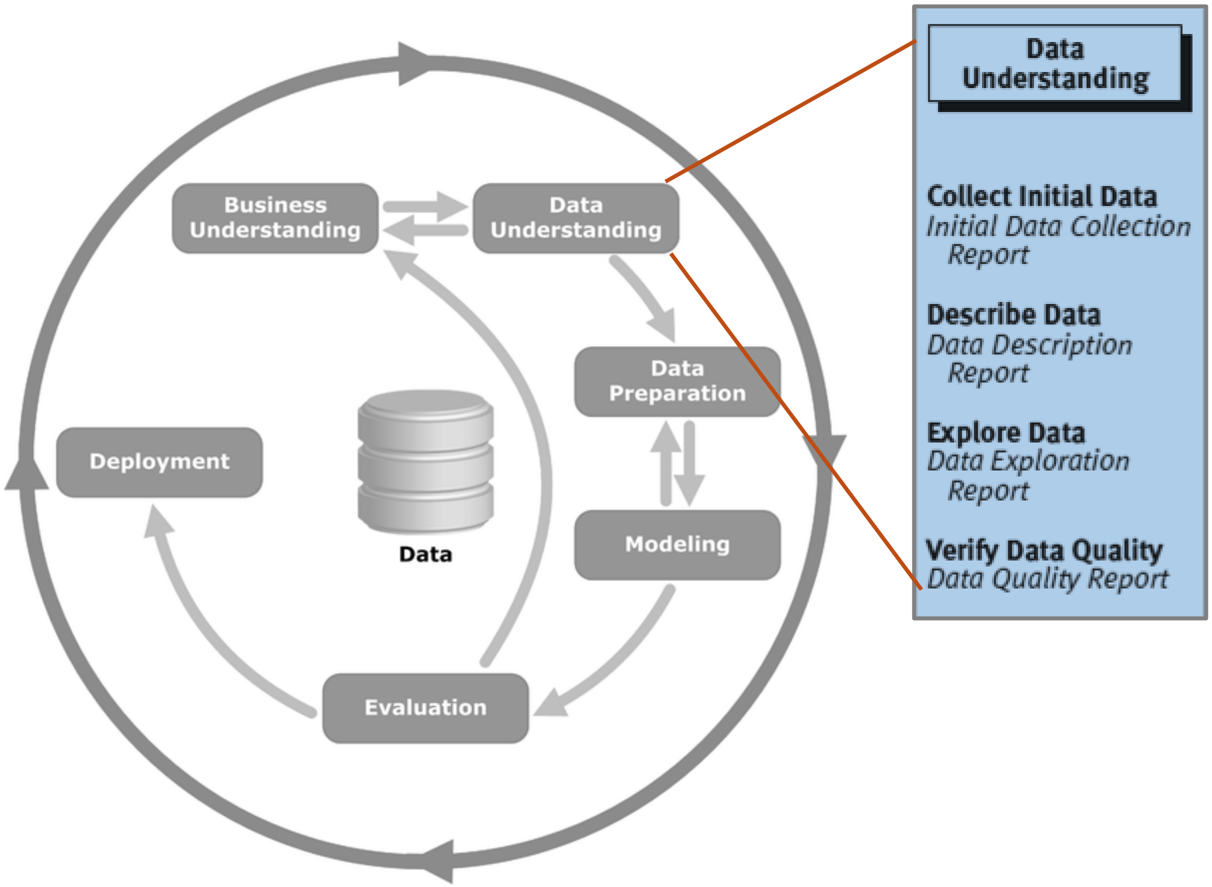
Based in Slides by Tan, Steinbach, Karpatne, Kumar

R Code Examples

- Available R Code examples are indicated on slides by the R logo

- The Examples are available at https://mhahsler.github.io/Introduction_to_Data_Mining_R_Examples/

Exploring Data in the Data Mining Process



Topics

- **Exploratory Data Analysis**
- Summary Statistics
- Visualization

What is Data Exploration?

“A preliminary exploration of the data to better understand its characteristics.”

- Key motivations of data exploration include
  - Helping to select the right tool for preprocessing or analysis
  - Making use of humans’ abilities to recognize patterns. People can recognize patterns not captured by data analysis tools

- Related to the area of Exploratory Data Analysis (EDA)
  - Created by statistician John Tukey
  - Seminal book is "Exploratory Data Analysis" by Tukey
  - A nice online introduction can be found in Chapter 1 of the NIST Engineering Statistics Handbook
  - http://www.itl.nist.gov/div898/handbook/index.htm

Topics

- Exploratory Data Analysis
- **Summary Statistics**
- Visualization

Summary Statistics

Summary statistics are numbers that summarize properties of the data

Summarized properties include location and spread for continuous data

Examples: location - mean
spread - standard deviation

Most summary statistics can be calculated in a single pass through the data

Categorical Features: Frequency and Mode

- The frequency of an attribute value is the percentage of time the value occurs in the data set
  - For example, given the attribute 'gender' and a representative population of people, the gender 'female' occurs about 60% of the time.

- The mode of an attribute is the most frequent attribute value

Continuous/Ordinal Features:
Measures of Location - Mean and Median

- The mean is the most common measure of the location of a set of points.
- However, the mean is very sensitive to outliers.
- Thus, the median or a trimmed mean is also commonly used.

$$\text{mean}(x) = \overline{x} = \frac{1}{m}\sum_{i=1}^{m} x_i$$

$$\text{median}(x) = \begin{cases} x_{(r+1)} & \text{if } m \text{ is odd, i.e., } m = 2r+1 \\ \frac{1}{2}(x_{(r)} + x_{(r+1)}) & \text{if } m \text{ is even, i.e., } m = 2r \end{cases}$$

Robust against outliers

Measures of Spread: Range and Variance

- Range is the difference between the max and min
- The variance or standard deviation is the most common measure of the spread of a set of points.

$$\text{variance}(x) = s_x^2 = \frac{1}{m-1}\sum_{i=1}^{m}(x_i - \overline{x})^2$$

- Other measures are often used.

$$\text{AAD}(x) = \frac{1}{m}\sum_{i=1}^{m}|x_i - \overline{x}|$$

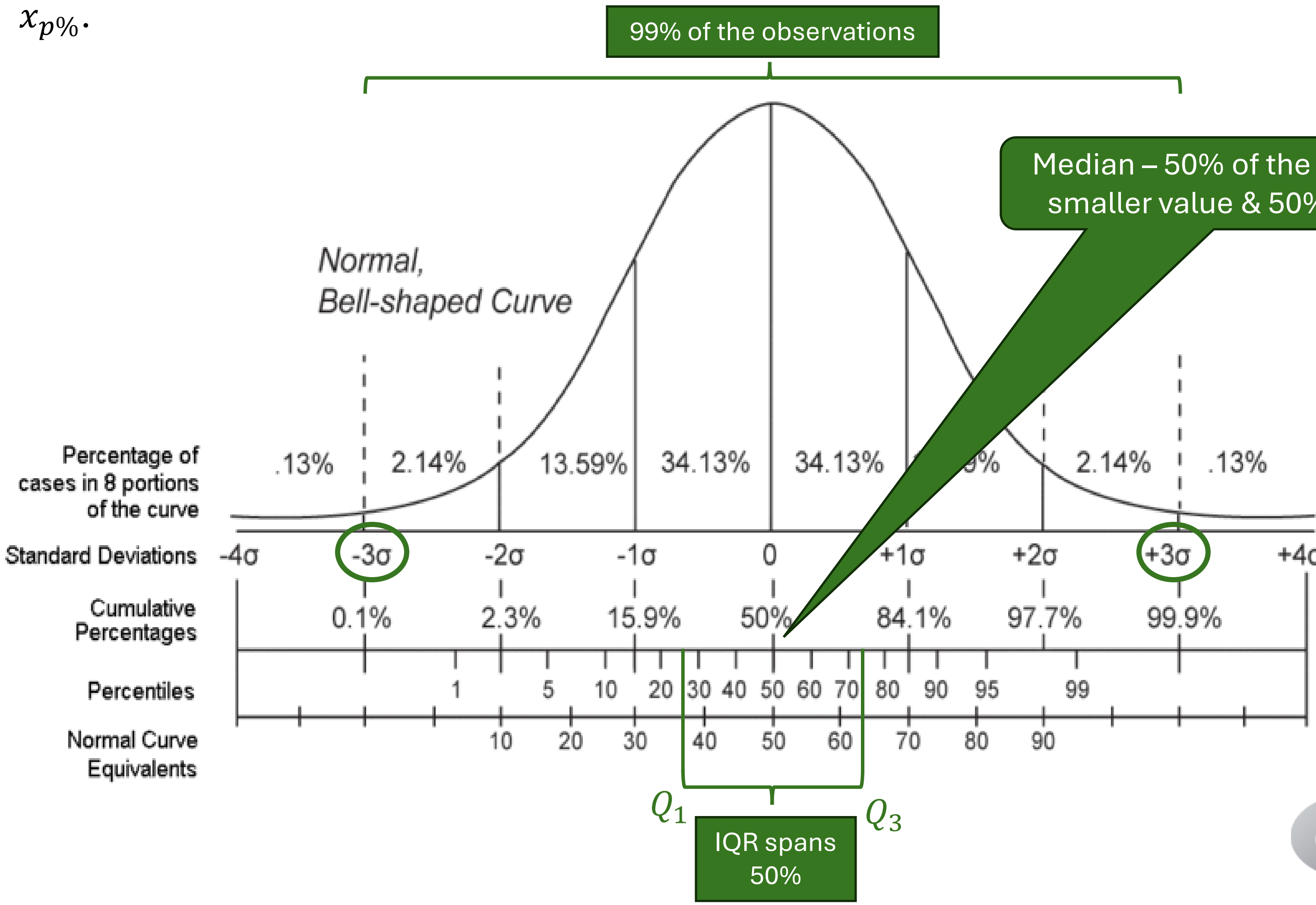
$$\text{MAD}(x) = median\left(\{|x_1 - \overline{x}|, \ldots, |x_m - \overline{x}|\}\right)$$

$$\text{IQR interquartile range}(x) = x_{75\%} - x_{25\%}$$

Robust against outliers

Percentiles of a Distribution

- Given an ordinal or continuous attribute x and a number p between 0 and 100, the p^{th}percentile is a value $x_{p\%}$ of x such that p% of the observed values of x are less than $x_{p\%}$.



Pearson Correlation

- The Pearson correlation coefficient measures the (linear) relationship between two variables.
- To compute Pearson correlation (Pearson's Product Moment Correlation), we standardize data objects, p and q, and then take their dot product

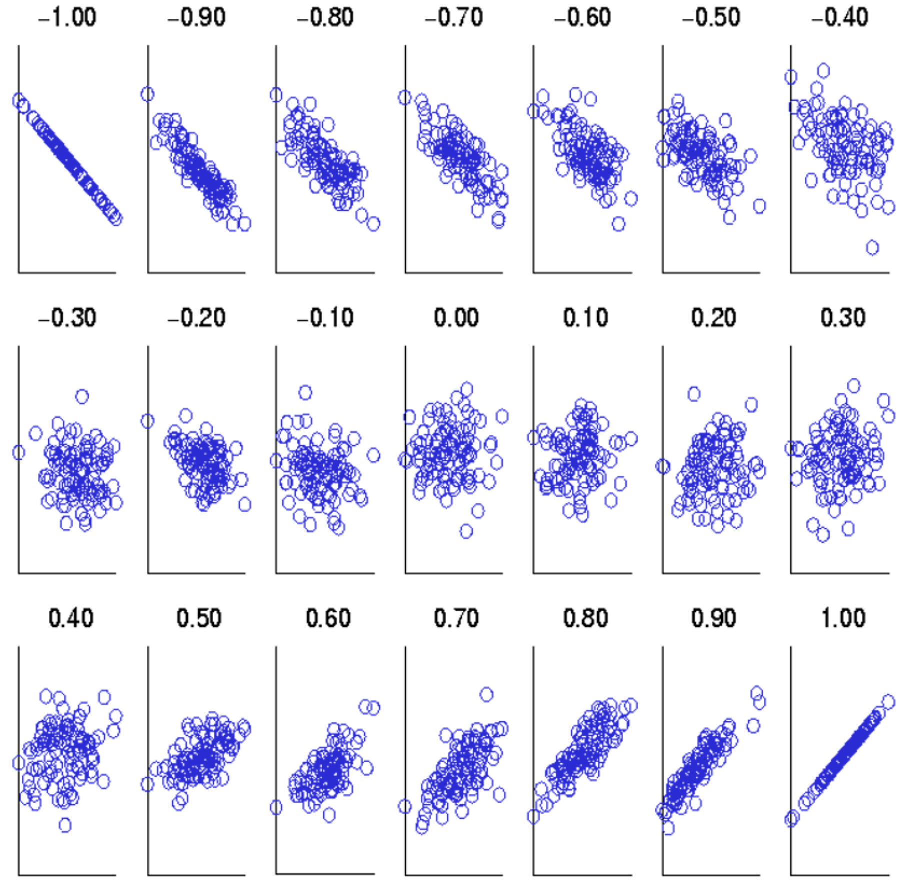
$$\rho = \frac{\mathrm{cov}(X, Y)}{\mathrm{sd}(X)\,\mathrm{sd}(Y)}$$

- Estimation:

$$r = \frac{\sum (x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum (x_i - \bar{x})^2 \sum (y_i - \bar{y})^2}}$$

- Correlation is often used as a measure of similarity.

Visually Evaluating Correlation



Scatter plots showing data with correlation from –1 to 1.

Rank Correlation

- Measure the degree of similarity between two ratings (e.g., ordinal data).
- Is more robust against outliers and does not assume normality of data or linear relationship like Pearson Correlation.
- Measures (all are between -1 and 1)
  - Spearman's Rho: Pearson correlation between ranked variables.
  - Kendall's Tau

$$\tau = \frac{N_s - N_d}{\frac{1}{2}n(n-1)}$$

N_s... concordant pair
N_d... discordant pair

  - Goodman and Kruskal's Gamma

$$\gamma = \frac{N_s - N_d}{N_s + N_d}$$

Topics

- Exploratory Data Analysis
- Summary Statistics
- **Visualization**

Visualization

Visualization is the conversion of data into **a visual or tabular** format so that the characteristics of the data and the **relationships among data items or attributes** can be analyzed or reported.

Visualization of data is one of the most powerful and appealing techniques for data exploration.

Humans have a well-developed ability to analyze large amounts of information that is presented visually

- Can detect general patterns and trends
- Can detect outliers and unusual patterns

Representation

- Is the mapping of information to a visual format
- Data objects, their attributes, and the relationships among data objects are translated into graphical elements such as **points, lines, shapes, and colors**.

- Examples:
  - —Objects are often represented as points.
  - —Their attribute values can be represented as the position of the points or the characteristics of the points, e.g., color, size, and shape.
  - —If position is used, then the relationships of points, i.e., whether they form groups or a point is an outlier, is easily perceived.

Arrangement

- Is the placement of visual elements within a display
- Can make a large difference in how easy it is to understand the data

Example:

	1	2	3	4	5	6
1	0	1	0	1	1	0
2	1	0	1	0	0	1
3	0	1	0	1	1	0
4	1	0	1	0	0	1
5	0	1	0	1	1	0
6	1	0	1	0	0	1
7	0	1	0	1	1	0
8	1	0	1	0	0	1
9	0	1	0	1	1	0

	6	1	3	2	5	4
4	1	1	1	0	0	0
2	1	1	1	0	0	0
6	1	1	1	0	0	0
8	1	1	1	0	0	0
5	0	0	0	1	1	1
3	0	0	0	1	1	1
9	0	0	0	1	1	1
1	0	0	0	1	1	1
7	0	0	0	1	1	1

The Iris Dataset

Many of the exploratory data techniques are illustrated with the Iris Plant data set.

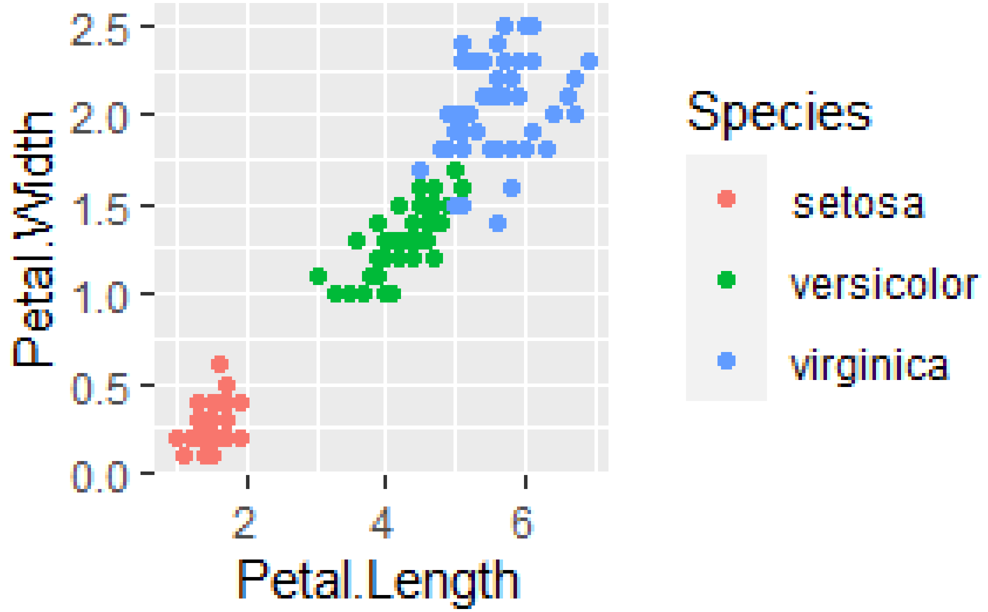
- Included as a demo datasert in many tools (R, scikit-learn, Rapidminer, …).
- Can be obtained from the UCI Machine Learning Repository http://www.ics.uci.edu/~mlearn/MLRepository.html
- From the statistician R.A. Fisher
- 150 flowers, three types (classes).
- Four (non-class) attributes

	Sepal.Length	Sepal.Width	Petal.Length	Petal.Width	Species
1	5.1	3.5	1.4	0.2	setosa
2	4.9	3.0	1.4	0.2	setosa
3	4.7	3.2	1.3	0.2	setosa

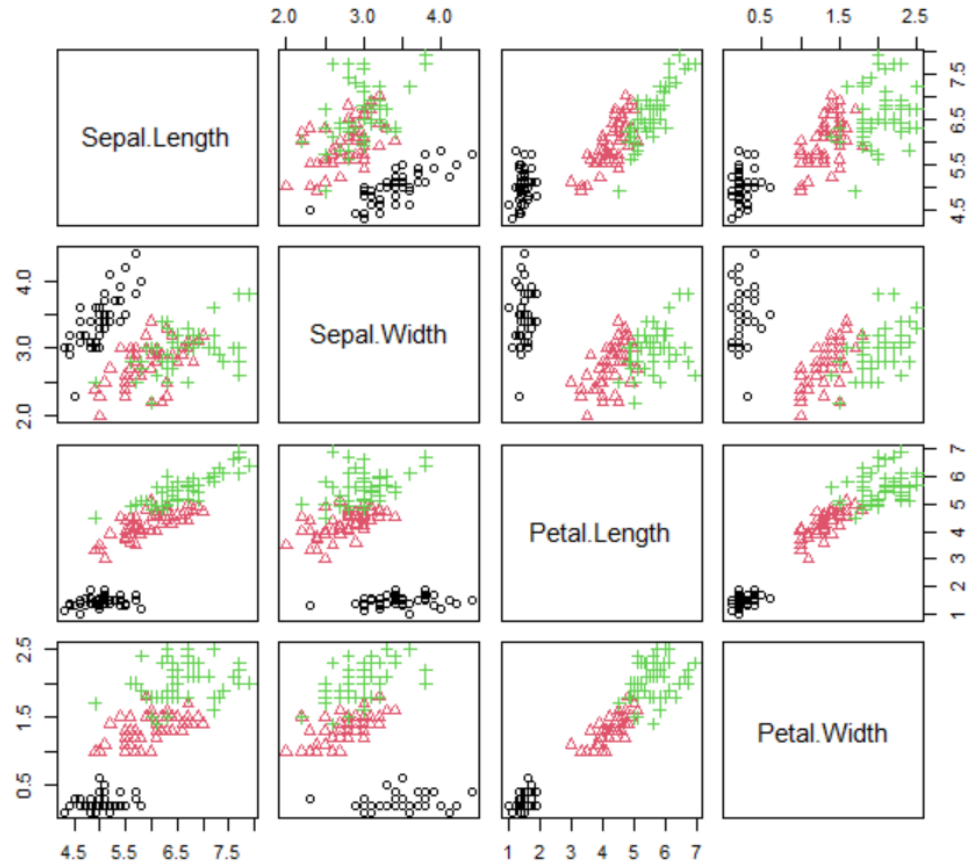
…

Scatter Plots

- Attributes values determine the position
- Two-dimensional scatter plots most common, but can have three-dimensional scatter plots
- Often additional attributes can be displayed by using the size, shape, and color of the markers that represent the objects



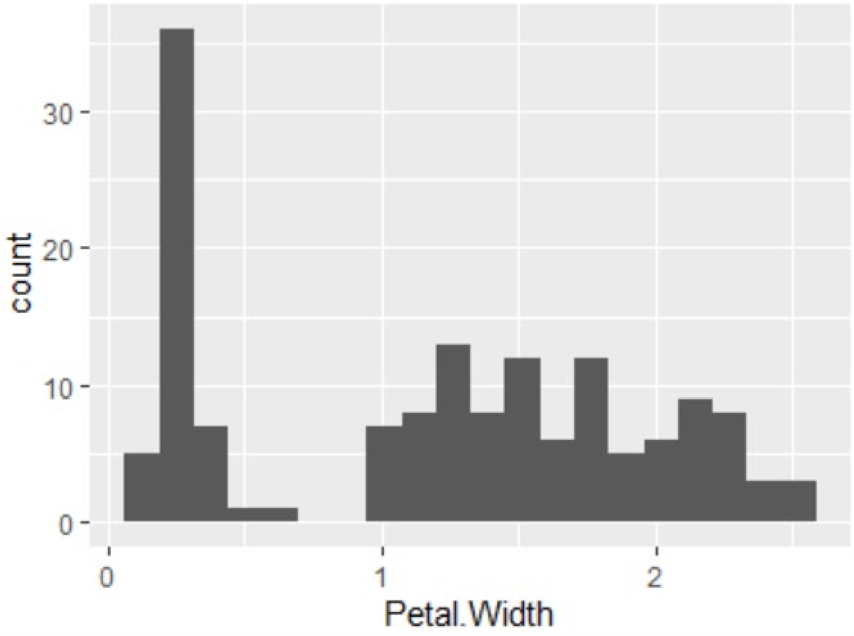
Scatter Plot Array of Iris Attributes

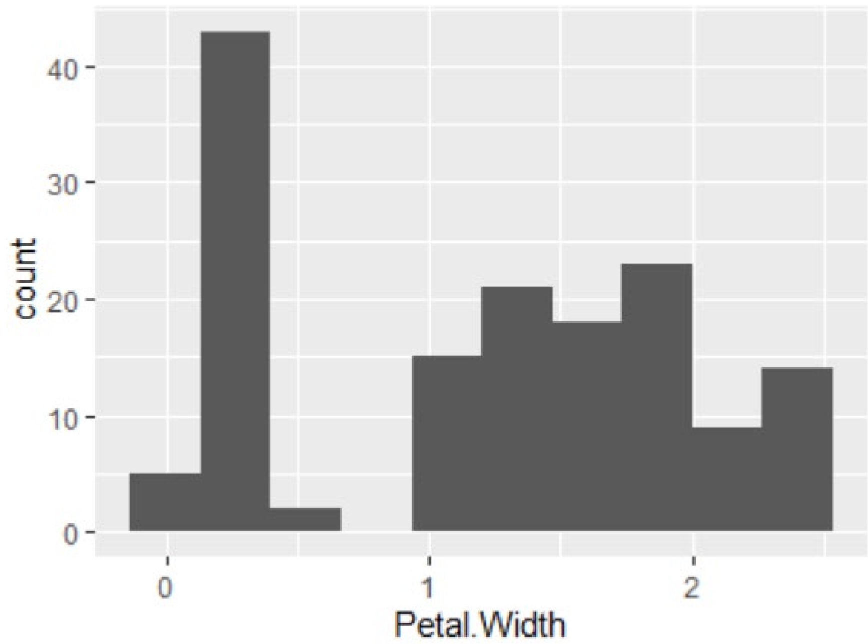


Distribution: Histograms

- Usually shows the distribution of values of a single variable
- Divide the values into bins and show a bar plot of the number of objects in each bin.
- The height of each bar indicates the number of objects
- Shape of histogram depends on the number of bins
- Kernel-based density estimation (KDE) can be used to smooth histograms.

Example: Petal Width (10 and 20 bins, respectively)





Distribution Box Plots

- Invented by J. Tukey as a simplified version of a PDF/histogram that is robust against outliers.
- Used to compare distributions.

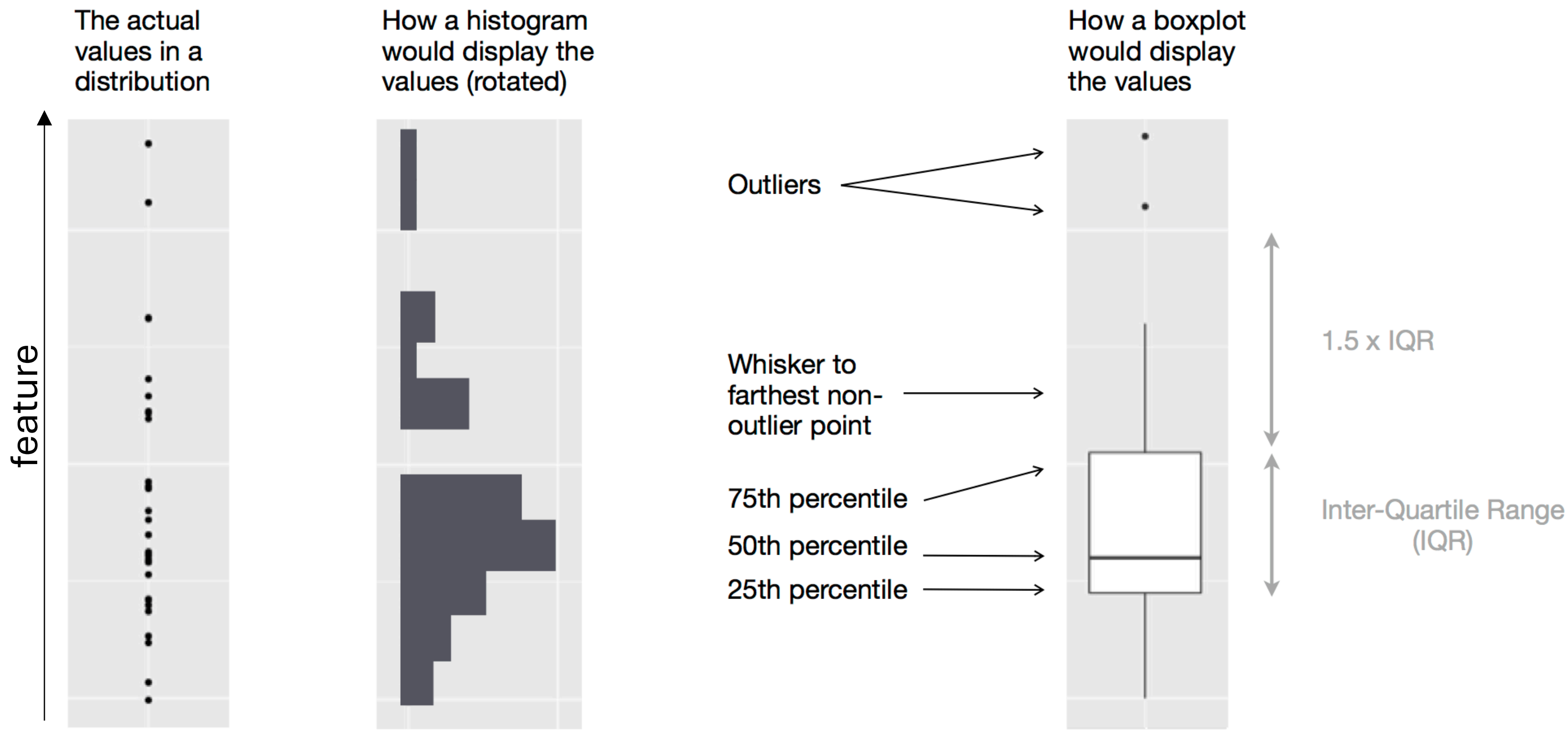
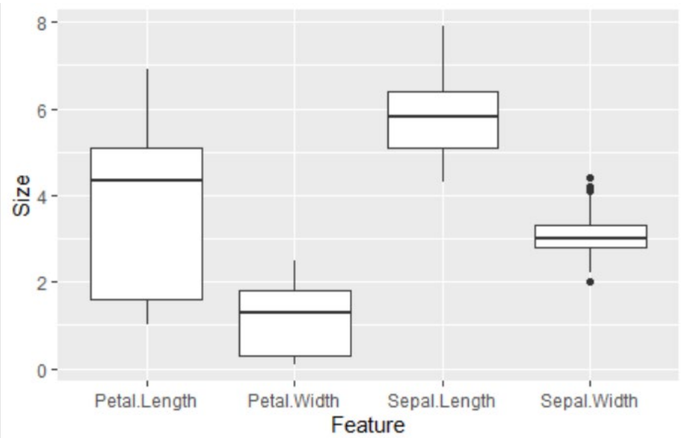


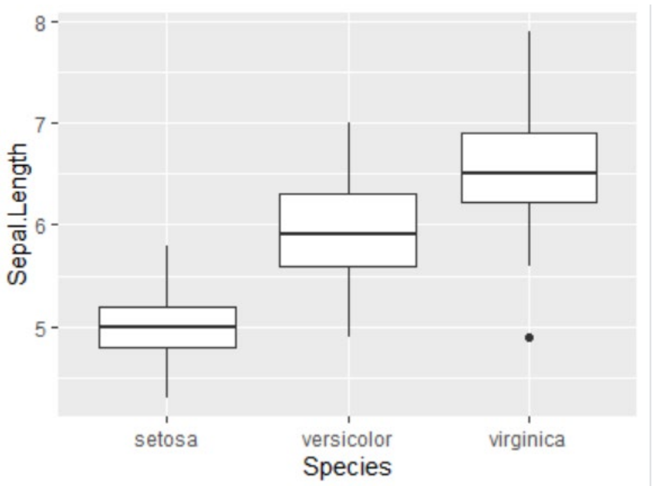
Figure source: [Data visualization – R for Data Science (2e)]

Examples of Box Plots

- Box plots can be used to compare the distribution of attributes or subgroups.

	Sepal.Length	Sepal.Width	Petal.Length	Petal.Width	Species
1	5.1	3.5	1.4	0.2	setosa
2	4.9	3.0	1.4	0.2	setosa
3	4.7	3.2	1.3	0.2	setosa

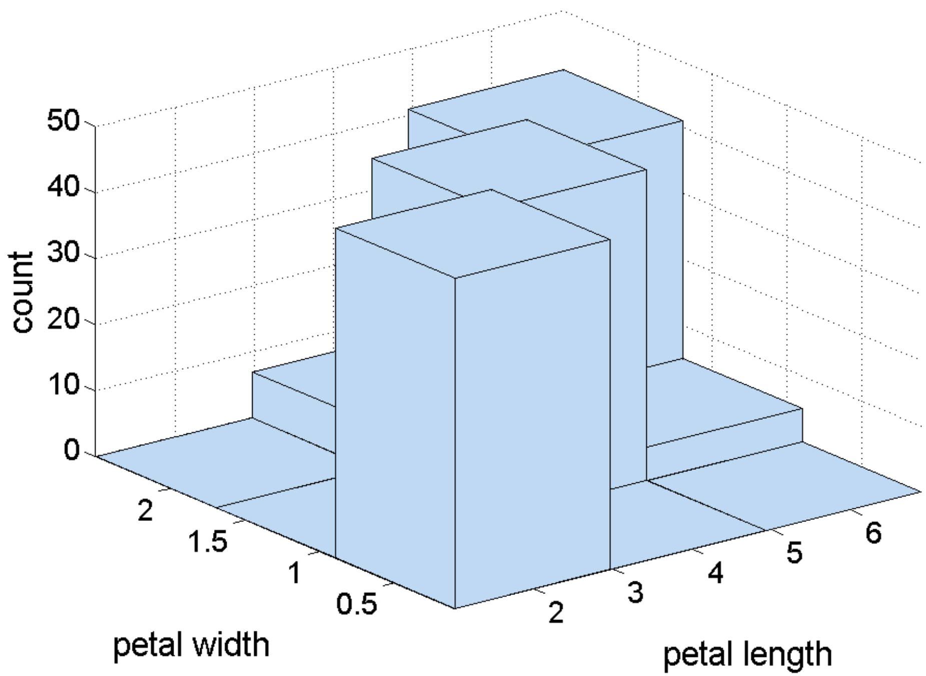




Two-Dimensional Histograms

- Show the joint distribution of the values of two attributes

Example: petal width and petal length. What does this tell us?

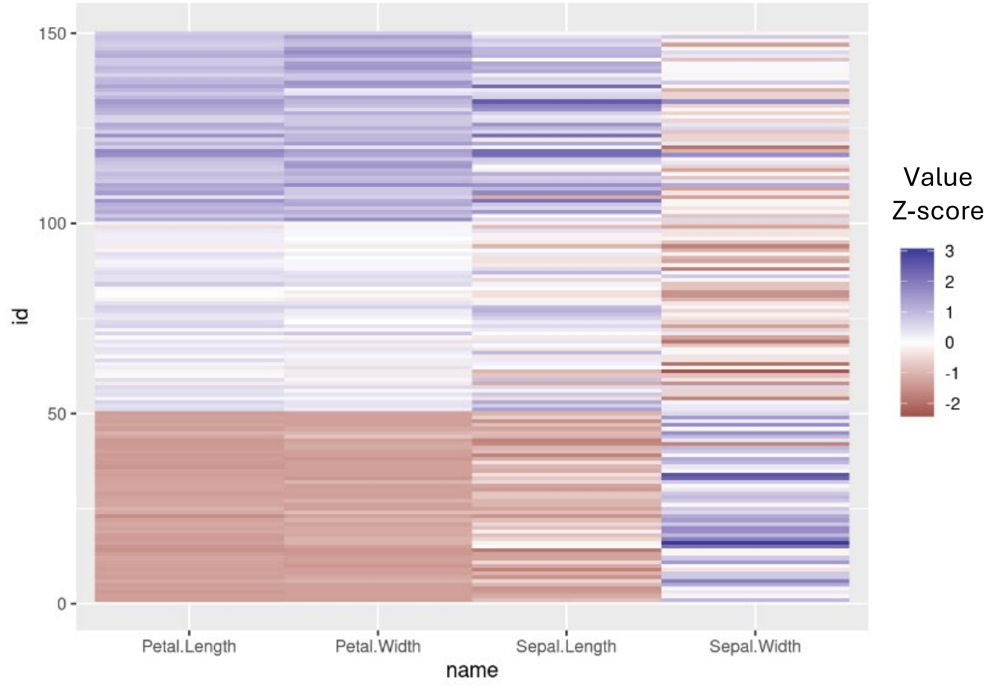


Note: Matrix visualizations are often preferred.

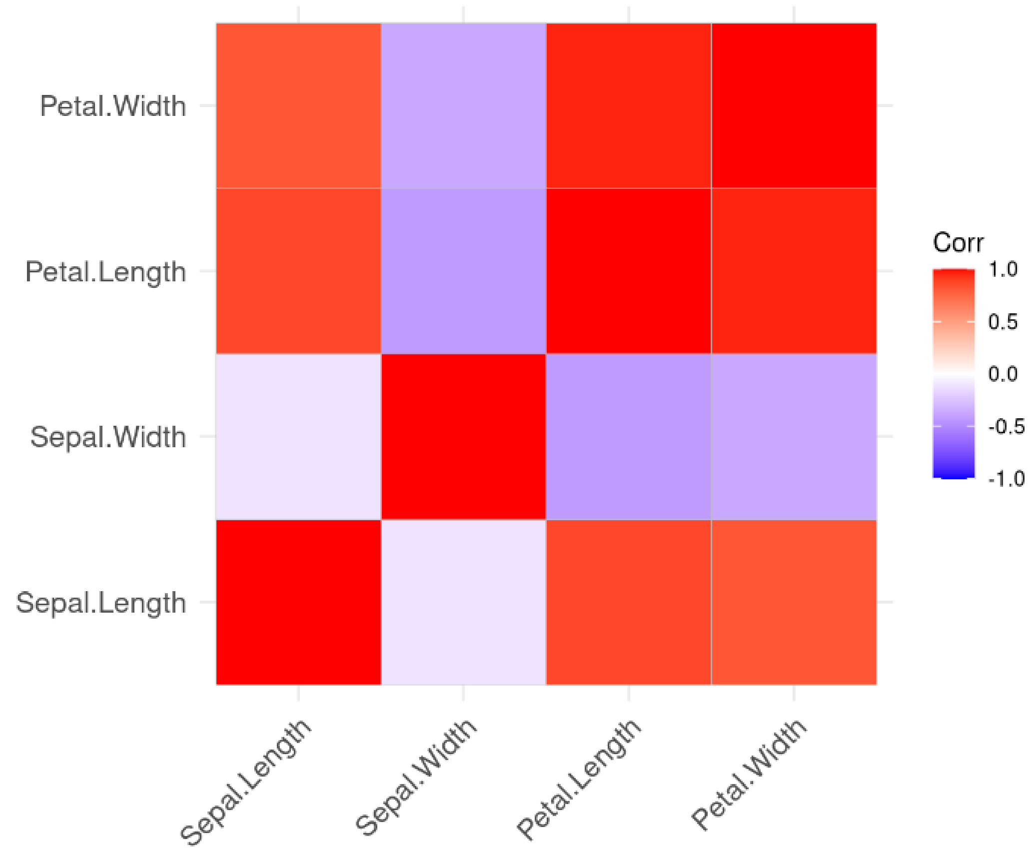
Matrix Plots

- Can plot a data matrix
- Can be useful when objects are sorted according to class
- Typically, the attributes are normalized to prevent one attribute from dominating the plot
- Plots of similarity or distance matrices can also be useful for visualizing the relationships between objects

Example: The Iris Data Matrix



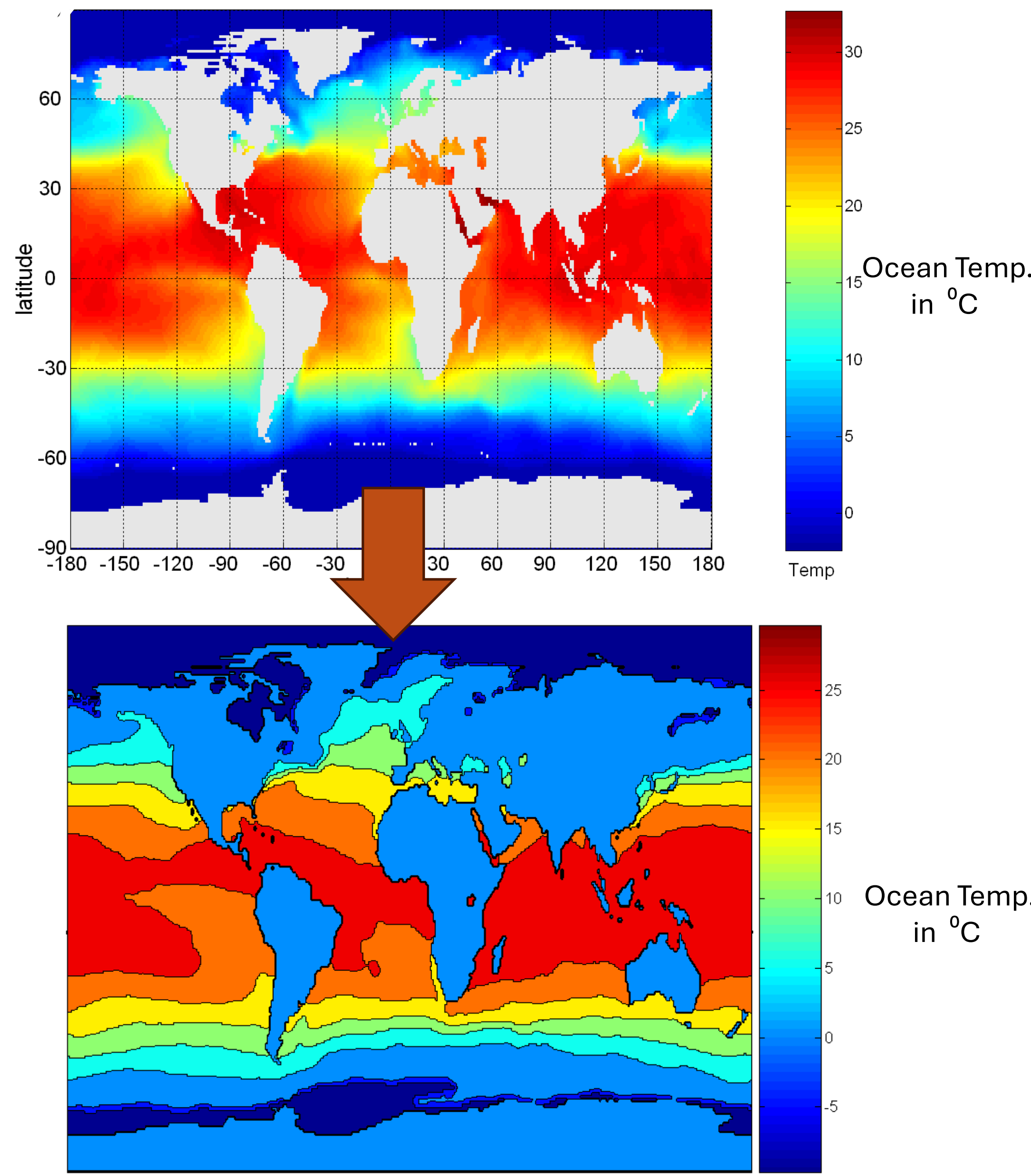
Matrix plot example: The Iris Correlation Matrix



Contour Plots

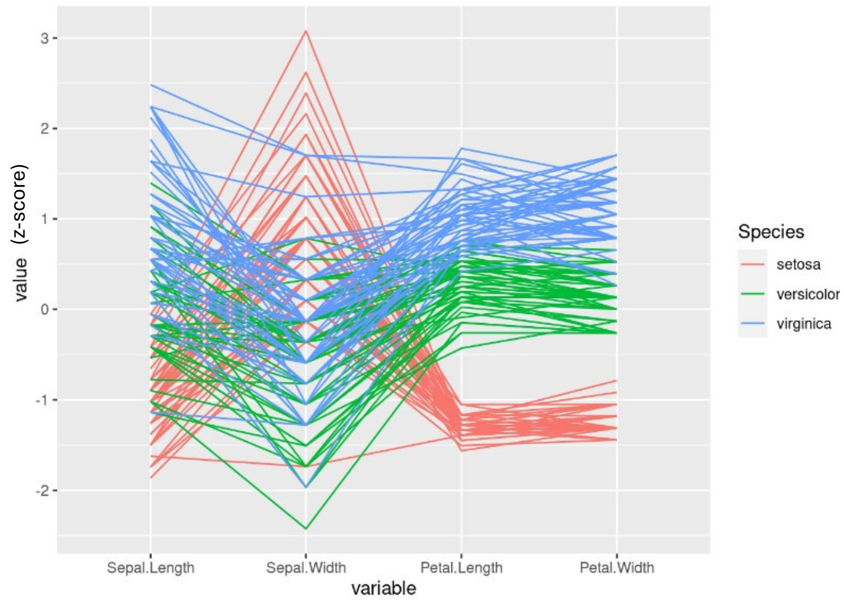
- Useful when a continuous attribute is measured on a **spatial grid**
- They partition the plane into regions of similar values
- The contour lines that form the boundaries of these regions connect points with equal values
- The most common example is contour maps of elevation
- Can also display temperature, rainfall, air pressure, etc.

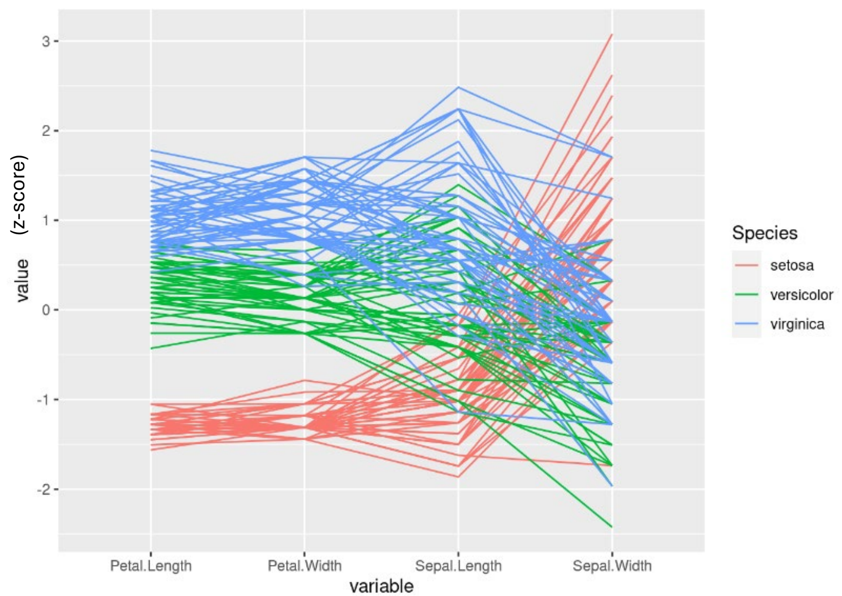
Sea Surface Temperature (SST) for July 1982



Parallel Coordinates

- Used to plot the attribute values of high-dimensional data
- Instead of using perpendicular axes, use a set of parallel axes
- The attribute values of each object are plotted as a point on each corresponding coordinate axis and the points are connected by a line
- Thus, each object is represented as a line
- Often, the lines representing a distinct class of objects group together, at least for some attributes
- Ordering of attributes is important in seeing such groupings





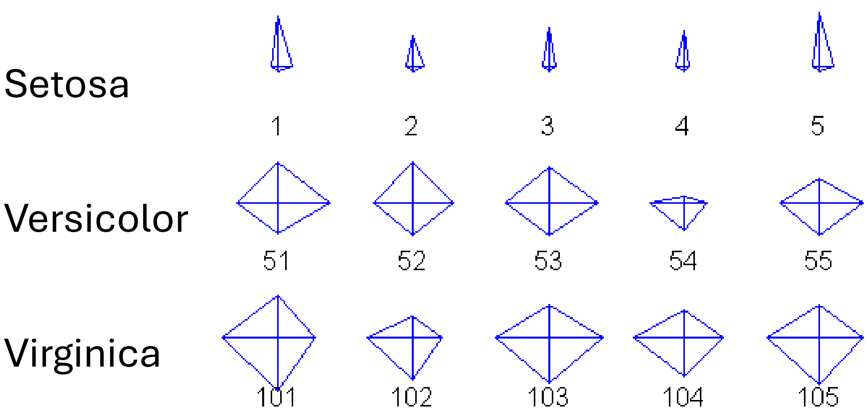
Reordered features

Other Visualization Techniques

- Translate each feature to a feature (a length or size) of a glyph.

Also called radar charts

Star Plots



Chernoff Faces

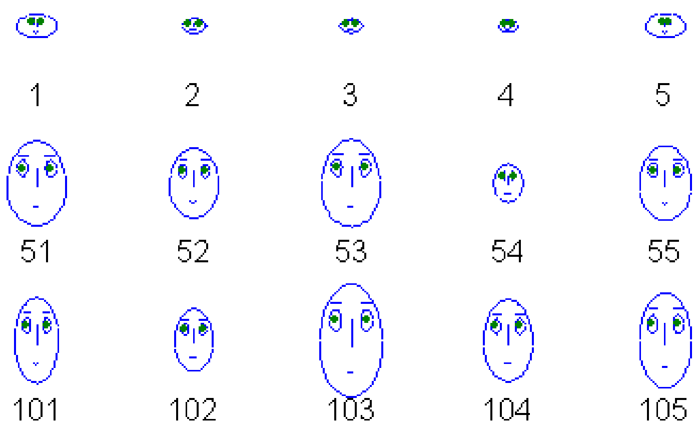
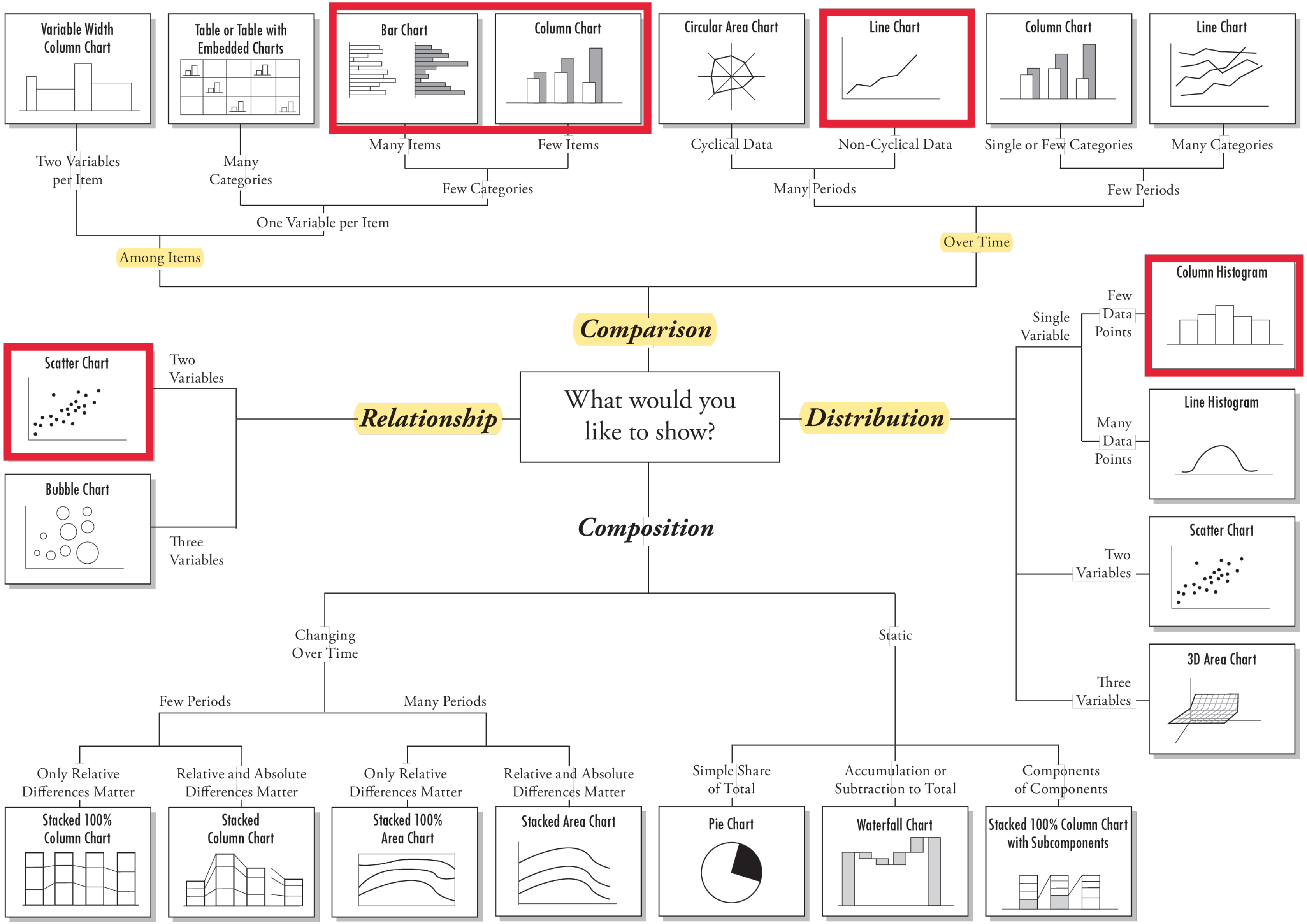


Chart Suggestions—A Thought-Starter



www.ExtremePresentation.com

Conclusion

- Exploring data is the first step when working with data.
- The goal is to:
  1. Understand what data is available.
  2. Assess data distributions and how variables relate to each other.
  3. Assess data quality.

- Understanding the data is necessary to decide on data preparation and modeling.