Exploratory Data Analysis

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Introduction Exploratory Data Analysis

- Graphics and Exploratory Data Analysis
 - Classical Data Analysis vs. EDA
 - Box plot
 - Histogram
 - ECDF plot
 - Run chart
 - Lag plot
 - Scatter plot
 - Q-Q plot
 - ROC curves

Reading Material

- Books:
 - P.Cohen, Empirical Methods for Artificial Intelligence, MIT Press, 1995
- Websites:
 - Engineering Statistics Handbook at NIST (www.itl.nist.gov/div898/handbook/eda/eda.htm)
 - An Introduction to R graphics (https://www.stat.auckland.ac.nz/~paul/RGraphics/ chapter1.pdf)
 - Galery of Data Visualization (http://euclid.psych.yorku.ca/SCS/Gallery/)

Exploratory Data Analysis (EDA)

- ► EDA is an approach to analyse data that employs various techniques to :
 - Find structure in the data
 - Extract relevant variables
 - Detect outliers and anomalies
 - Test underlying assumptions

Exploratory Data Analysis (EDA)

► EDA vs. Classical Data Analysis

EDA:

- The focus is on the data
- ► Find structure and outliers
- Find models suggested by the data
- It is based on graphical techniques

Classical:

- The focus is on the model
- Estimate parameters of the model
- Generate predicted values from the model
- It uses statistical tests and regression models

Exploratory Data Analysis (EDA)

► EDA vs. Classical Data Analysis

EDA:

- No or few assumptions on the data
- ► It is suggestive, indicative and subjective

Classical:

- It depends on underlying assumptions (e.g. normality)
- It is rigorous, formal and objective

► A classical example*

Group 1		Group 2		Group 3		Group 4	
X	Y	X	Y	X	Y	X	Y
10.00	8.04	10.00	9.14	10.00	7.46	8.00	6.58
8.00	6.95	8.00	8.14	8.00	6.77	8.00	5.76
13.00	7.58	13.00	8.74	13.00	12.74	8.00	7.71
9.00	8.81	9.00	8.77	9.00	7.11	8.00	8.84
11.00	8.33	11.00	9.26	11.00	7.81	8.00	8.47
14.00	9.96	14.00	8.10	14.00	8.84	8.00	7.04
6.00	7.24	6.00	6.13	6.00	6.08	8.00	5.25
4.00	4.26	4.00	3.10	4.00	5.39	19.00	12.50
12.00	10.84	12.00	9.13	12.00	8.15	8.00	5.56
7.00	4.82	7.00	7.26	7.00	6.42	8.00	7.91
5.00	5.68	5.00	4.74	5.00	5.73	8.00	6.89

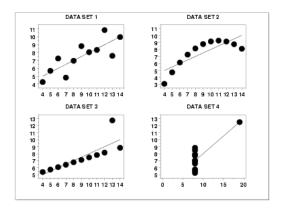
^{*} Taken from the Engineering Statistics Handbook website

Summary of data and best linear fit for Y as function of X (values are similar for all groups):

	Group 1	Group 2	Group 3	Group 4
N	11	11	11	11
Mean of X	9.0	9.0	9.0	9.0
Mean of Y	7.5	7.5	7.5	7.5
Intercept	3.0	3.0	3.0	3.0
Slope	0.5	0.5	0.5	0.5
Correlation	0.82	0.82	0.82	0.82

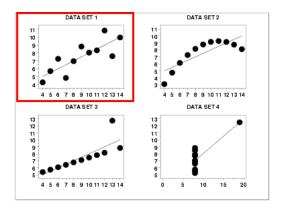
Conclusion: The four data sets look "equivalent"

Scatter plots:



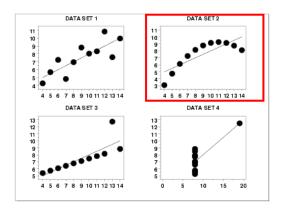
Conclusion: The four data sets do not look "equivalent".

Scatter plots:



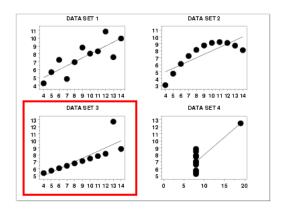
Conclusion: The first data set is linear with some scatter

Scatter plots:



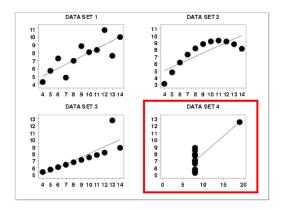
Conclusion: The second data set is non-linear

Scatter plots:



Conclusion: The third data set has an outlier

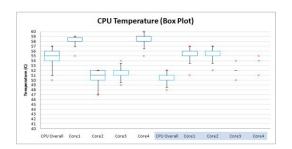
Scatter plots:



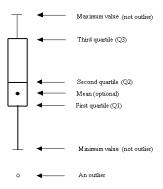
Conclusion: Bad experimental design in the fourth data set

- ▶ What to learn from the example?
 - Quantitative statistics are numerical summaries of the data
 - They focus on particular aspects of the data (location, association, etc.)
 - ► They are not right or wrong per se, but depend of the underlying assumptions.
 - Ex: applying linear regression to non-linear data (such as data set 2) may not be meaningful.
 - ► EDA, through the use of scatter plots, gave further insight into the data.

Find out the meaning!



▶ Box Plot



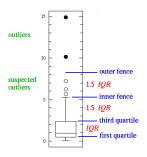
- Quartiles split data into quarters
- Interquartile range is

$$IQR = Q3 - Q1$$

Outliers are outside the interval

$$[Q1 - 1.5 \cdot IQR, Q3 + 1.5 \cdot IQR]$$

► Box Plot



Mild outliers are inside the intervals

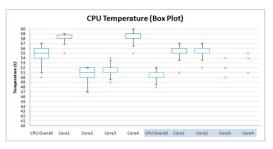
$$[Q3 + 1.5 \cdot IQR, Q3 + 3 \cdot IQR]$$

$$[Q1 - 3 \cdot IQR, Q1 - 1.5 \cdot IQR]$$

 Extreme outliers are outside the interval

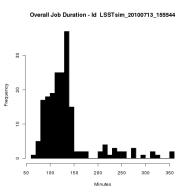
$$[Q1 - 3 \cdot IQR, Q3 + 3 \cdot IQR]$$

► Box Plot

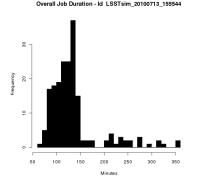


- Does the location differ between groups?
- Does the variation differ between groups?
- Are there any outliers?

► Find out the meaning!

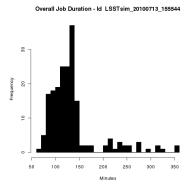


▶ Histogram



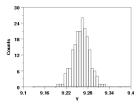
- Divide range into equal-sized bins
- Count the number of values that fall into each bin
- Divide the count in each bin by the total number of observations (optional)

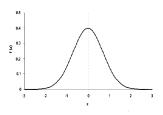
Histogram



- What kind of distribution do the data come from?
- Where are the data located?
- How spread out are the data?
- Are the data symmetric or skewed?
- ► Are there outliers in the data?

► Histogram

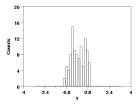


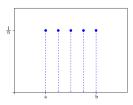


- Symmetric, moderated-tailed histogram (top plot)
- It suggests a normal distribution (bottom plot)

Next step: Check normality

Histogram

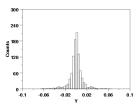


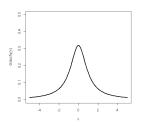


- Symmetric, short-tailed histogram (top plot)
- It suggests a uniform distribution (bottom plot)

Next step: Check if the data follows a uniform distribution

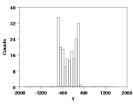
► Histogram

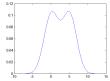




- Symmetric, long-tailed histogram (top plot)
- It suggests a Cauchy distribution (bottom plot)
- Next step: Check if the data follows a Cauchy distribution

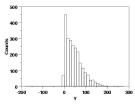
Histogram

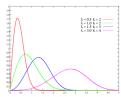




- Symmetric, bimodal histogram (top plot)
- It suggests a mixture of two distributions (bottom plot)

Histogram

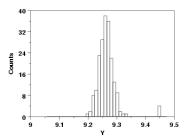




Right-skewed histogram (top plot)

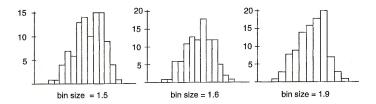
- It suggests an extreme-value distribution, e.g. Weibull (bottom plot)
- Same reasoning applies to left-skewed data

► Histogram



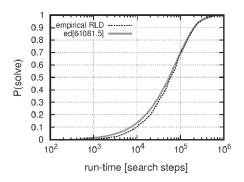
Data with outliers (in the right)

► Histogram

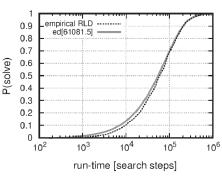


The size of the bins may affect the shape of the histogram!

Find out the meaning!

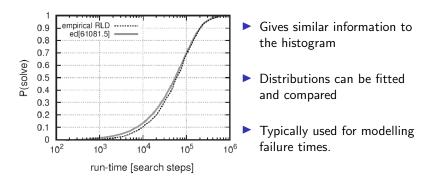


▶ Empirical Cumulative Distribution Function (ECDF) Plot

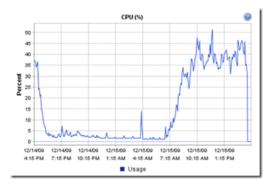


- Estimates $P(X \le x)$
- Sort the *n* values in increasing order
 - Plot the values in the x-axis, such that the *i*-th point is plotted on the y-axis at the values (i-1)/n and i/n.
- Connect the points with a staircase.

▶ Empirical Cumulative Distribution Function (ECDF) Plot



Find out the meaning!

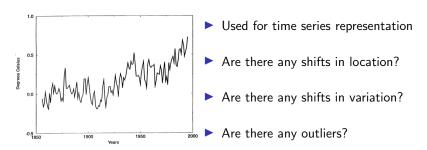


Run Chart

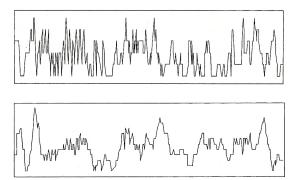


- Used for time series representation
- ► Are there any shifts in location?
- Are there any shifts in variation?
- ► Are there any outliers?

► Run Chart

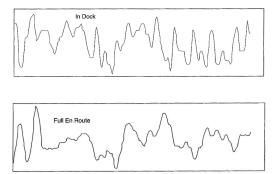


► Run Chart Example (Cohen 1995)



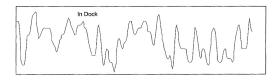
Run chart for the number of ships in dock (top) and full en route (bottom) over time.

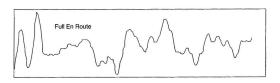
► Run Chart Example



Time series smoothing (e.g. averaging values in a time window)

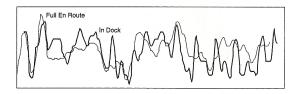
► Run Chart Example





Time series shifting

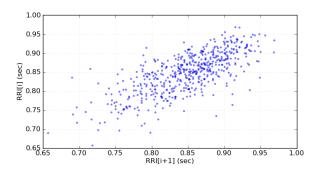
Run Chart Example



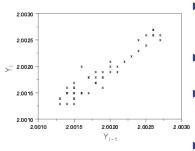
Time series overlapping: time series in dock antecipates the full en route series quite well.

The number of ships in dock predicts the number of ships en route in a few days.

► Find out the meaning!

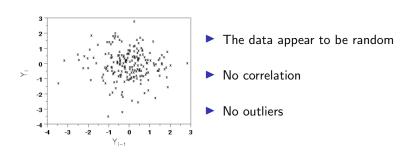


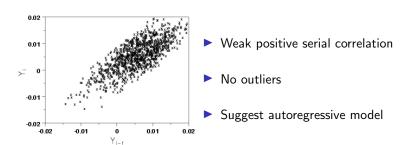
► Lag plot

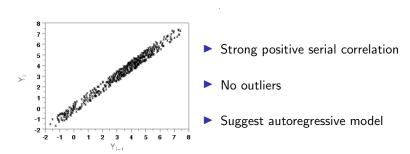


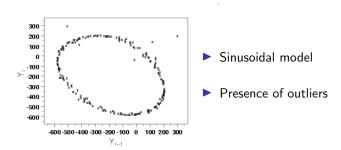
 Provides an indication of the randomness of a time series

- ▶ Do the data appear to be random?
- Is there serial correlation in the data?
- Are there outliers in the data?

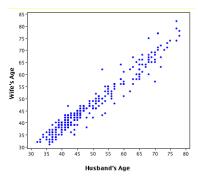




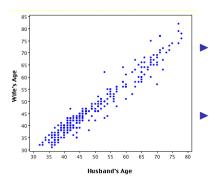




► Find out the meaning!



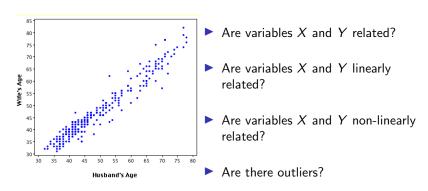
Scatter plot



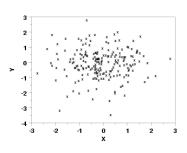
Plot of the values of Y against the corresponding values of X.

Useful to reveal relationships or association between two or more variables.

Scatter plot

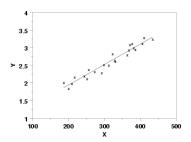


► Scatter Plot



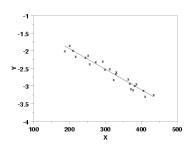
No relationship

Scatter Plot



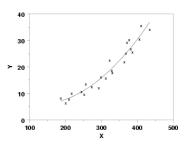
Strong linear relationship (positive correlation)

Scatter Plot



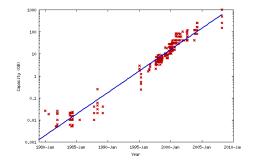
Strong linear relationship (negative correlation)

► Scatter Plot



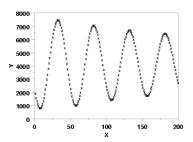
Quadratic relationship

Scatter Plot



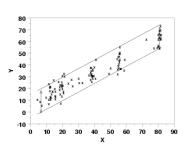
Exponential relationship (note the logarithm scale of the y axis)

► Scatter Plot



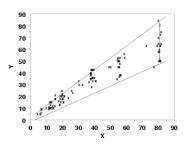
Sinusoidal relationship

Scatter Plot



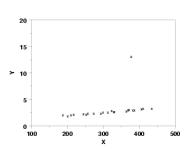
Linear relationship with constant variation

► Scatter Plot



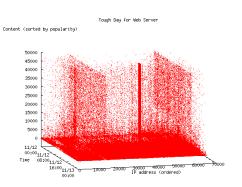
Linear relationship with non-constant variation

► Scatter Plot

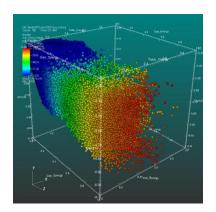


Linear relationship with an outlier

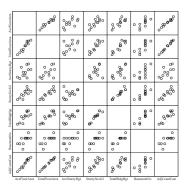
► A 3D Scatter plot



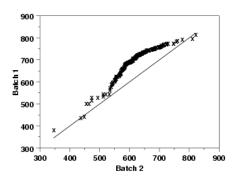
► A 4D Scatter plot



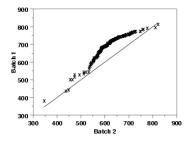
Scatter plot matrix



Find out the meaning!

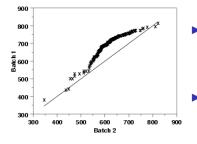


► Q-Q plot



- Plot quantiles of the first data set against the quantiles of the second data set
 - 45-degree reference line is plotted for reference

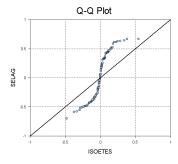
▶ Q-Q plot



Do two data sets come from populations with a common distribution?

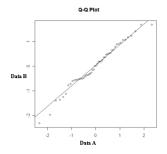
In this case, no

Q-Q plot



- Do two data sets come from populations with a common distribution?
- ► In this case, no

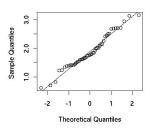
► Q-Q plot



- Do two data sets come from populations with a common distribution?
- In this case, maybe yes.
- Next step: Check with 2-sample K-S Test

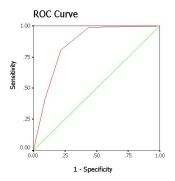
► Normal Q-Q plot

QPlot for the Log of the Carbon Monoxide

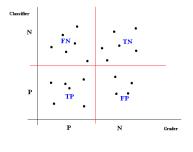


- Does the data set come from a population with a normal distribution?
- Most used way of checking normality before applying statistical tests
- A step further: Check normality with K-S Test

► Find out the meaning!



▶ ROC (Receiver Operating Characteristic) curves



 Evaluates the performance of classifiers with respect to a reference.

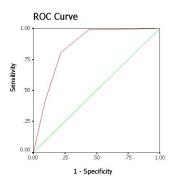
$$\blacktriangleright Sensitivity = \frac{TP}{TP+FN}$$

Specificity =
$$\frac{TN}{TN+FP}$$

Fall-out =
$$\frac{FP}{TN+FP}$$

= 1 - Specificity

ROC curves



- ROC curves are drawn as the discriminator threshold is varied
- ► The larger the area under the ROC curve, the better the classifier is
- Exception: if the ROC curves intersect each other, this is not so clear cut.

Other plots: Error Bar Plots

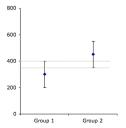
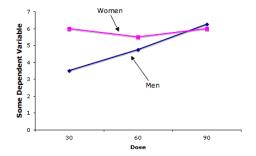


Figure 1: Mean reaction time (ms) and 95% confidence intervals for Group 1 (n=36) and Group 2 (n=34).

- ▶ Plots the means and some sort of error, e.g., confidence intervals (next lecture).
- Allows to detect significant differences between groups of observations.

Other plots: Interaction Plots



- ▶ Plots the means for each level of each factor (e.g., dose and gender).
- Allows to detect interaction between variables in an experimental design (next lecture).

Conclusions

- ► The main focus of EDA is on the data
- ► EDA relies strongly on graphical techniques to find structure and patterns in the data
- It suggests hypotheses to test
- Classical data analysis is still preferred as an ultimate step in research.