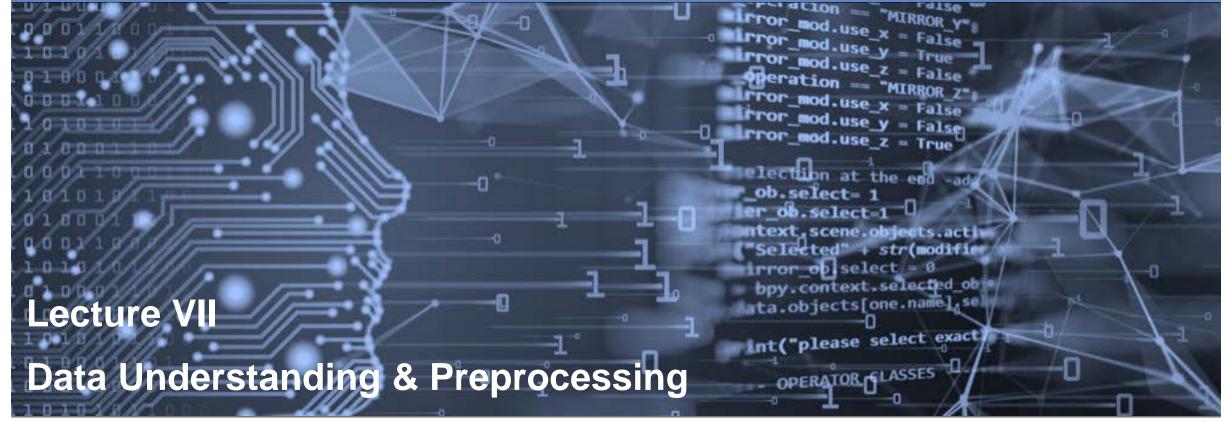
Machine Learning Applications



Winter semester 2019/2020
Henrik Simon & Sebastian Baumann

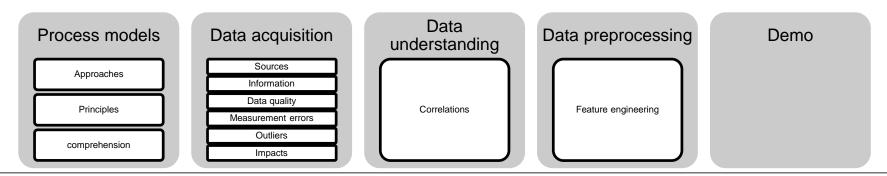




What should you be able to take out of the lecture today?



- What are important approaches for machine learning projects (process models, design principles)?
- When the use of the word prediction should be avoided (diagnosis vs. prognosis)?
- Why is business and data understanding important?
- How can we assess data quality and how can we trust data?
- How to deal with outlier and measurement uncertainties? What are negative influences?
- Why correlation analyses can be useful, but should be avoided?
- How can we extract and select meaningful predictors for modeling?





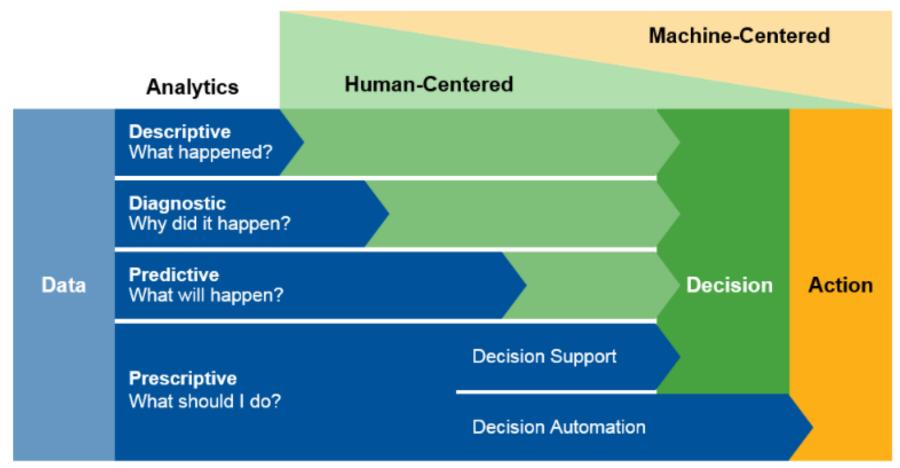


RECAP: PROCESS MODELS AND MACHINE LEARNING APPROACH



The four analytic capabilities of business intelligence: delivering hindsight, insight and foresight



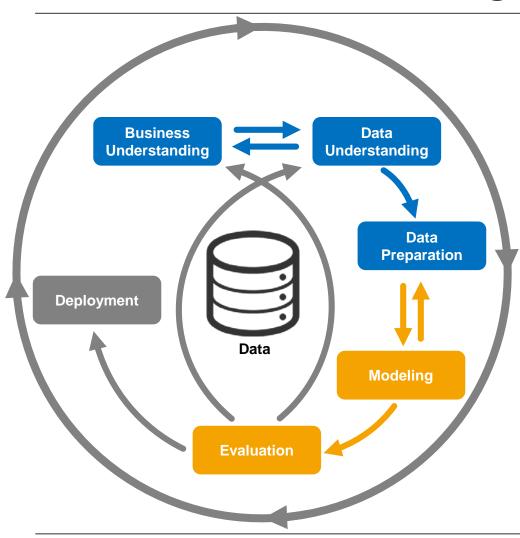


Source: Gartner Inc. [Publ.]: 2017 Planning Guide for Data and Analytics. Technical Professional Advice, G00311517 (2016)



Business Understanding and Data Understanding form the basis of a data mining / machine learning cycle.





Business Understanding

- initial phase that focuses on understanding the project objectives and requirements from a business perspective
- converting this knowledge into a data mining problem definition and a preliminary plan designed to achieve the objectives
- defines a clear objective and research question. What do you want to realize?
 Clustering, Classification, Regression | Diagnosis vs. Prognosis

Data Understanding

- based on an initial data collection; activities to get familiar with the data, to identify data quality problems, to discover first insights or to detect interesting subsets to form hypotheses for hidden information
- takes major influences on all following steps (GIGO: garbage in garbage out)
- definition and proof of data requirements

Data Preparation

- covers all activities to construct the final dataset from raw data, time consuming (50%-70%)
- devoting adequate energy to business understanding and data understanding can minimize this effort

Source: https://www.ibm.com/support/knowledgecenter/en/SS3RA7_15.0.0/com.ibm.spss.crispdm.help/crisp_overview.htm



Deeper look into CRISP-DM process steps



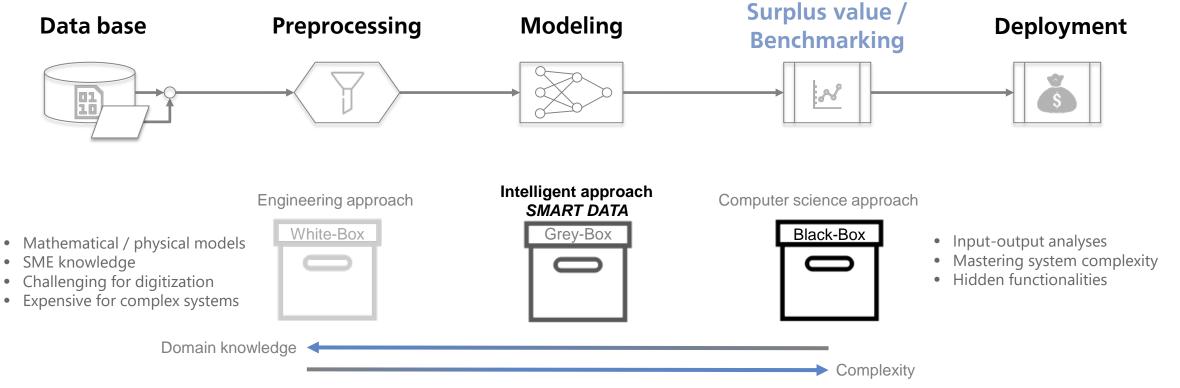
Business Objectives Background Business Objectives Business Success	Collect Initial Data Initial Data Collection Report	Data Set Data Set Description	Select Modeling	Evaluate Results	Dian Daniannana
Situation Assessment Inventory of Resources Requirements, Assumptions, and	Describe Data Data Description Report Explore Data Data Exploration Report Verify Data Quality Data Quality Report	Select Data Rationale for Inclusion / Exclusion Clean Data Data Cleaning Report Construct Data Derived Attributes Generated Records Integrate Data Merged Data Format Data Reformatted Data	Technique Modeling Technique Modeling Assumptions Generate Test Design Test Design Build Model Parameter Settings Models Model Description Assess Model Model Assessment Revised Parameter Settings	Assessment of Data Mining Results w.r.t. Business Success Criteria Approved Models Review Process Review of Process Determine Next Steps List of Possible Actions Decision	Plan Deployment Deployment Plan Plan Monitoring and Maintenance Monitoring and Maintenance Plan Produce Final Report Final Report Final Presentation Review Project Experience Documentation

Source: Pete Chapman, The CRISP-DM User Guide https://s2.smu.edu/~mhd/8331f03/crisp.pdf



Design principles





- Objection: optimization of model efforts (time, money, resources, accuracy) benchmarks are obligatory
- Correlation ≠ Causality
- Derivation of explainable AI / ML frameworks



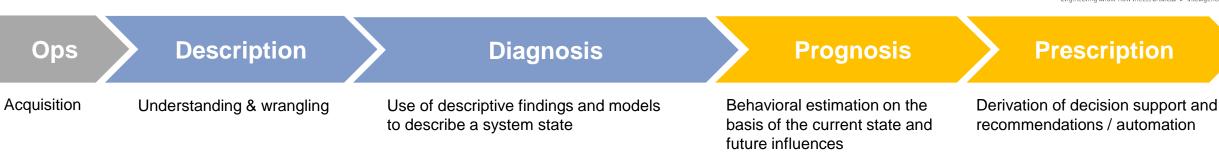


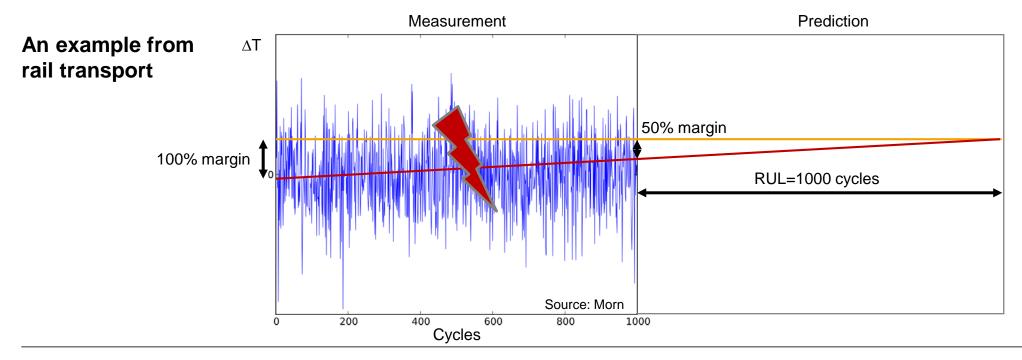
DIAGNOSIS VS. PROGNOSIS



The different capabilities provide a distinction between diagnosis and prognosis.









The different capabilities provide a distinction between diagnosis and prognosis.



Ops

Description

Diagnosis

Prognosis

Prescription

Acquisition

Understanding & wrangling

Use of descriptive findings and models to describe a system state

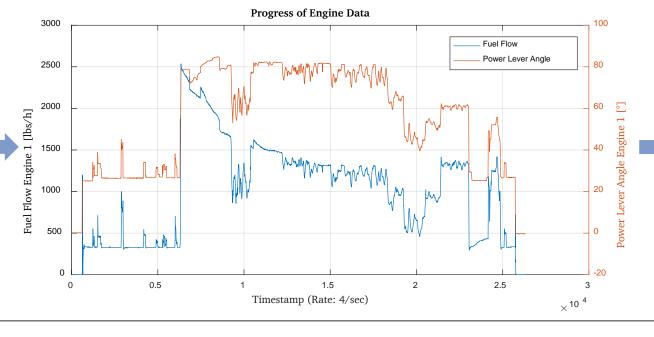
Behavioral estimation on the basis of the current state and future influences

Derivation of decision support and recommendations / automation





Source: karlenepetitt.blogspot.com



Predictable predictor? Predictive capability?



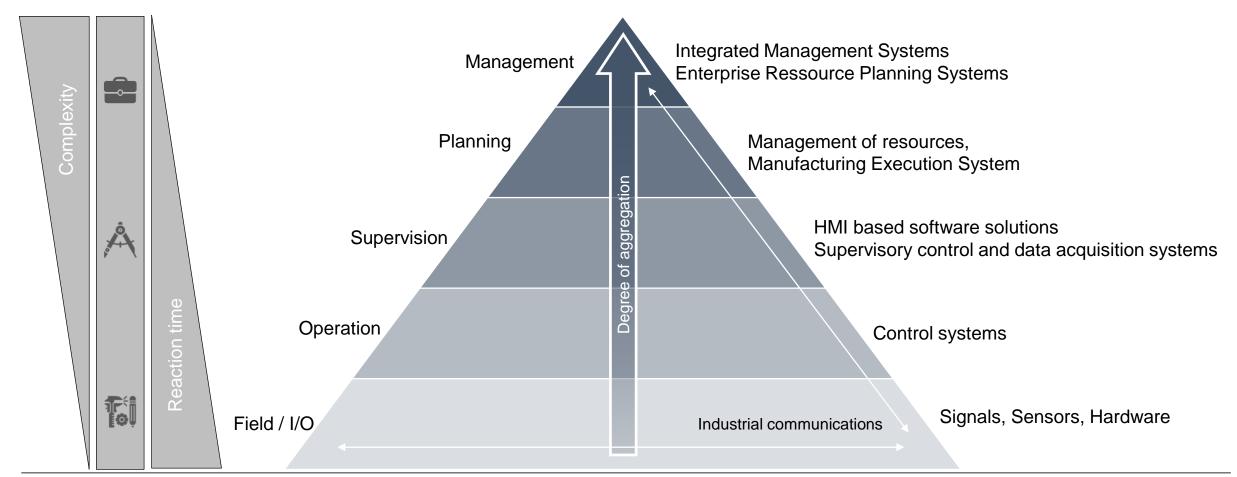


DATA ACQUISITION



Various automation levels lead to different information that can have the same data origin.



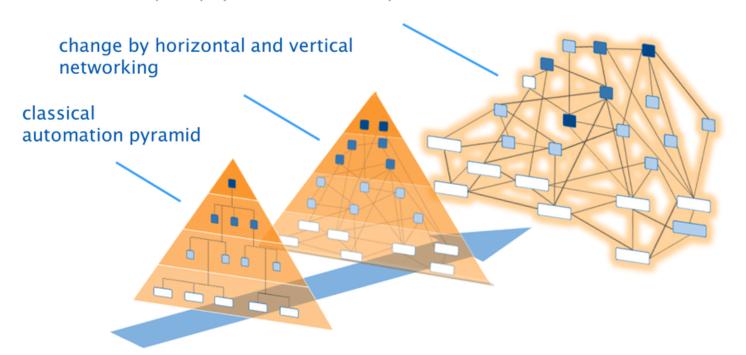


Future: Cyber physical systems based automation

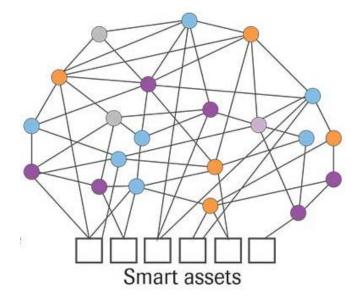
Vertical & horizontal integration



cyber-physical Production Systems (CPPS)



Automation services



Sources: Lipinski, Richter, Reiff-Stephan: Intelligent sensor systems for self-optimising production chains. In: Proceedings of the 1th Int. Conf. and Exh. on Future RFID Technologies. pp. 115–125 (2014); Labs: Industry 4.0 network architecture relies on interconnectivity, Online: https://www.foodengineeringmag.com/articles/97066-industry-40-network-architecture-relies-on-interconnectivity (2017)





DATA QUALITY



Assessing data quality

How to create trust and confidence



Definition Data quality

Data are of high quality if they are suitable for their intended use in operations, for decision support and for the planning of those.

Definition Meta Data

Structured information, which describes, explains, localizes, or simplifies in another way the fetch, usage or management of an information source.

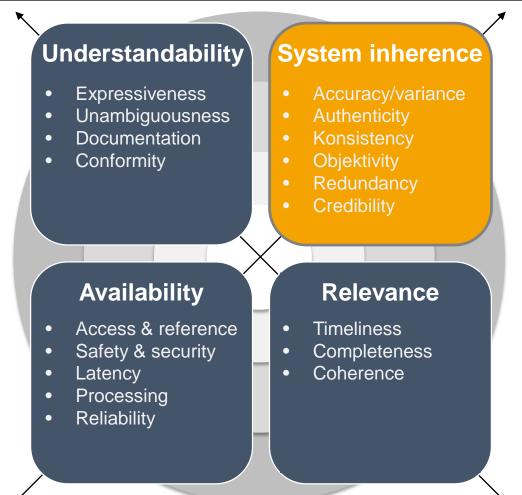
Data quality Information content Model quality Trust & confidence



Assessing the data quality

Classes and dimensions for data quality assessment





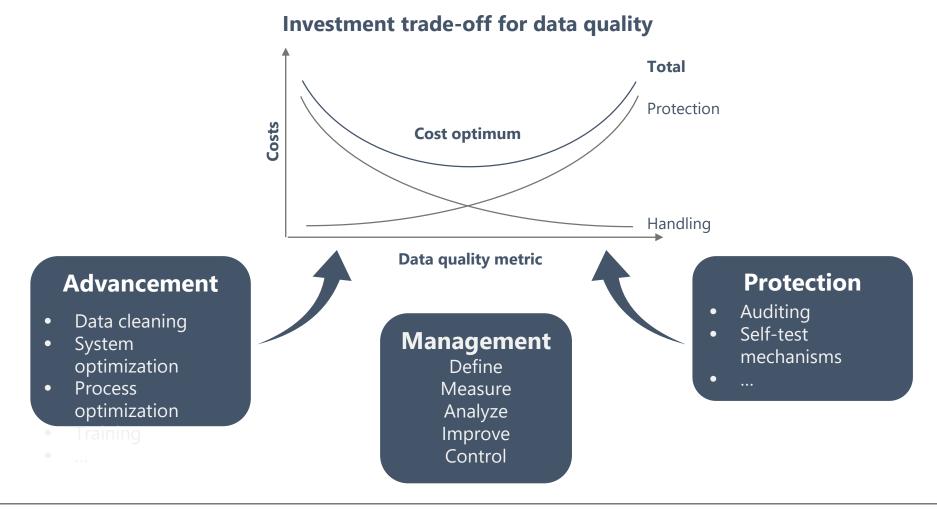
Area of high data quality



Assessing the data quality

Classes and dimensions for data quality assessment







MEASUREMENT ERRORS

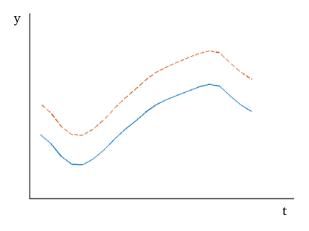


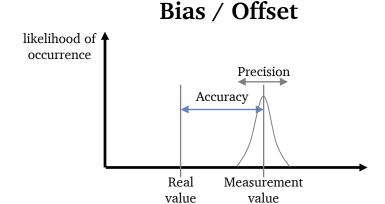
Illustration of measurement errors

Errors can be classified into three types that can overlap.

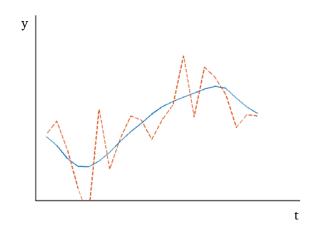


Systematic errors





Random errors

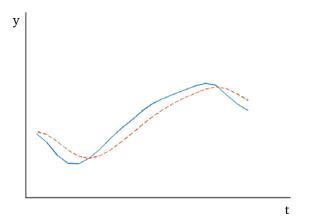


Variance

Signal to noise ratio (SNR)

$$\frac{P_{Signal}}{P_{Noise}} = 10^{\frac{SNR}{10 \, dB}}$$

Dynamic errors



Lag / Delay

Delay 1st order

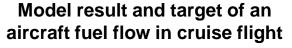
$$G(s) = \frac{1}{1 + Ts}$$

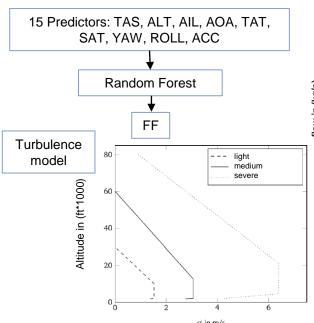


Measurement errors have a significant influence on the model quality of machine learning models.

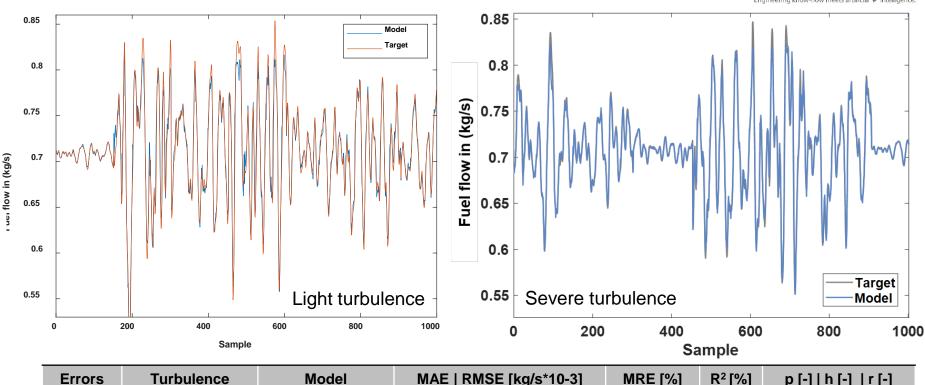








Performance metrics for models trained with original and manipulated data

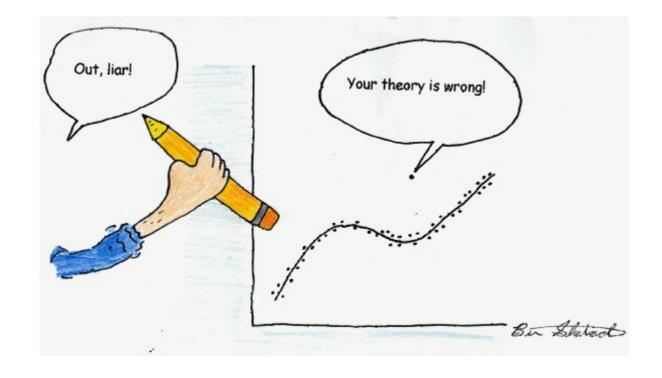


Errors	Turbulence	Model	MAE RMSE [kg/s*10-3]	MRE [%]	R ² [%]	p [-] h [-] r [-]
-	-	Original	.3 1.8	.04	99.01	
dyn. & stoch	Light	Manipulation	6.4 10.3	.9	95.84	<.01 1
	Medium	Manipulation	4.2 6.8	.6	98.31	0.84
	Severe	Manipulation	4.4 7.4	.62	97.96	





OUTLIER

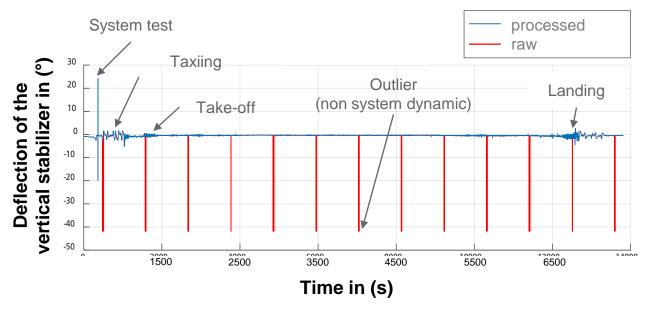


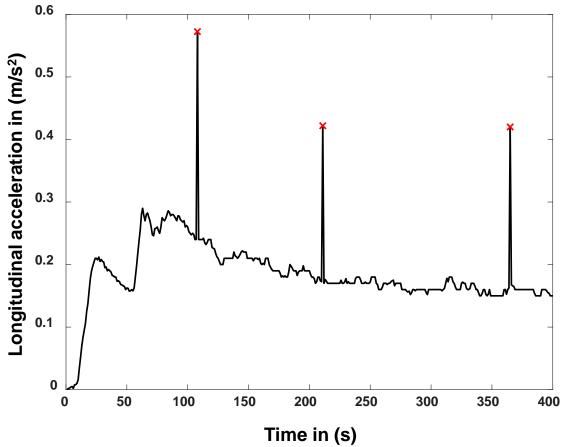


Outliers distort the system dynamic characteristic.



- Time series can contain non-system dynamic data points.
- Assessments turn out to be difficult
- Characteristics can be distorted by outliers





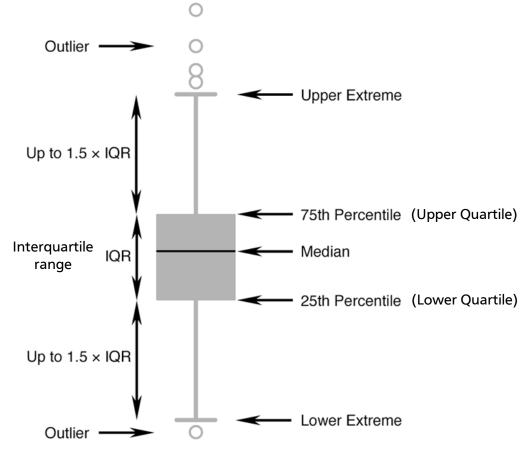


There is no unambiguous mathematical / physical description of outliers.



- Outliers stand out clearly from the time series
- Outliers are conspicuously far away from a measure of location (e. g. mean, median, interquartile distance)
- 5-point descriptions often only serve as an informal test

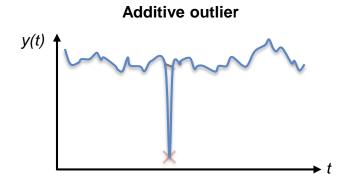
Boxplot according TUKEY

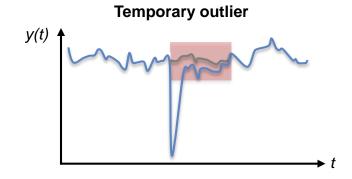


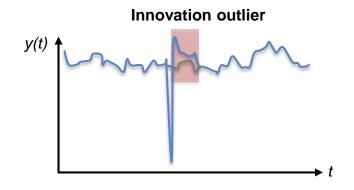
Tukey, J. W.: Exploratory Data Analysis. Pearson Publishing, Cambridge (1977) Picture Source: https://www.infragistics.com/community/blogs/b/tim_brock/posts/demystifying-box-and-whisker-plots-part-1

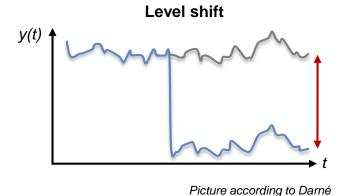
Sorts of outliers according to Aguinis













Examples for identification strategies



Median / Hampel filter

- Window width and threshold (variance / standard deviation) as settings
- Distance evaluation according to

$$|x_i - \widetilde{x_i}| > n_\sigma \sigma_i$$

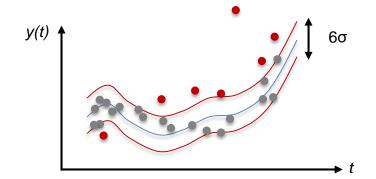
DFFITS

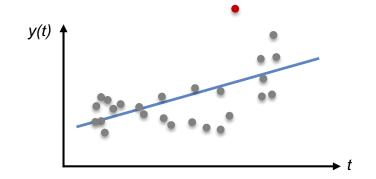
- Identification of influential data points on a regression model
- Outlier dimension with

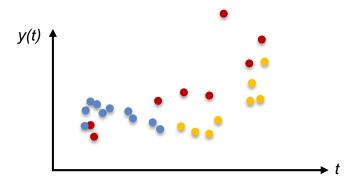
$$DFFITS_i = \frac{y - y_{(i)}}{\sigma_{(i)} \sqrt{h_{ii}}}$$

k-means

- E.g. calculation of first-degree differences
- Initialization of k cluster centers
- Iterative assignment of data points to clusters based on distances of the firstdegree differences
- Distance dimension between cluster centers as quality functional





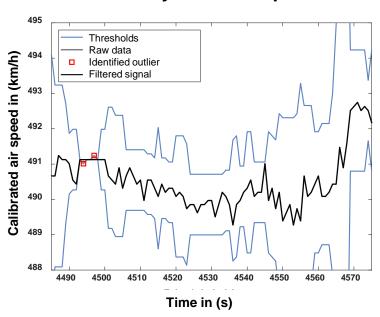




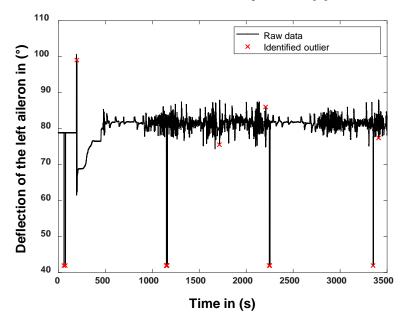
The assessment of system dynamics and outlier identification in time series is not trivial.



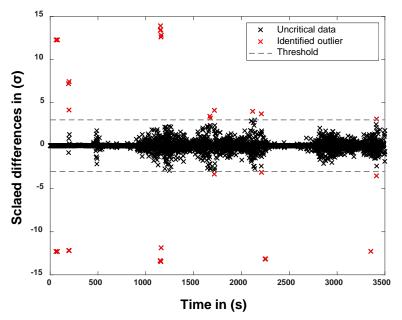
Sensitivity of the Hampel filter



Identified outlier of a hybrid approach



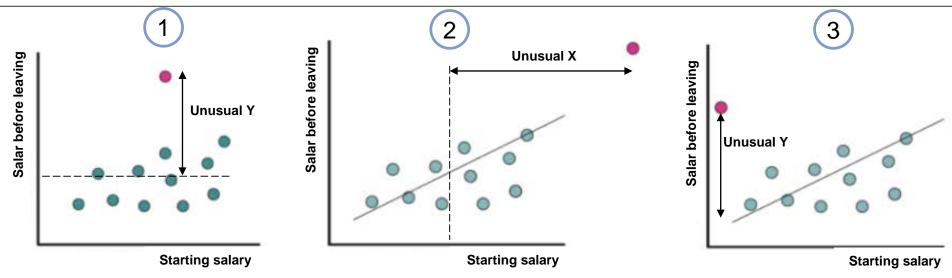
Identified outlier in the differences





Effects of outliers on statistical tests of more verifiable data.





Impacts on

- Slope (Effect Size): Type 3 outliers have a large impact on the estimated effect size
- Standard Error of Regression: Type 1 and 3 outliers increase the standard error of regression significantly
- P-Value: Type 1 outliers increase the p-value, 2 reduces it in a misleading way, and 3 has a wild and unpredictable effect on the p-value.

FSŔ)



INFLUENCES OF INSUFFICIENT DATA QUALITY



Bias-Variance-Trade-Off



Underfitting

Model is unable to capture the global behavior or pattern of the data. Possible causes: less amount of data, linear modeling with nonlinear data.

Overfitting

Model complexity approaches the complexity of training data, e. g. captures noise in data.

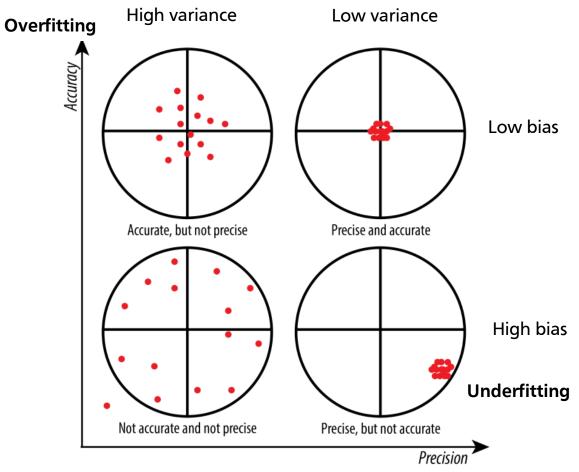
■ Bias-Variance-Trade-Off

mean approximation of the data

- simple models: bias to generalized data behavior
- complex models: Variance increases on test data

Generalizability

A model is over adjusted by agent A, if agent A* describes the training data worse with a larger error but the overall distribution of the data with a smaller error better than A.

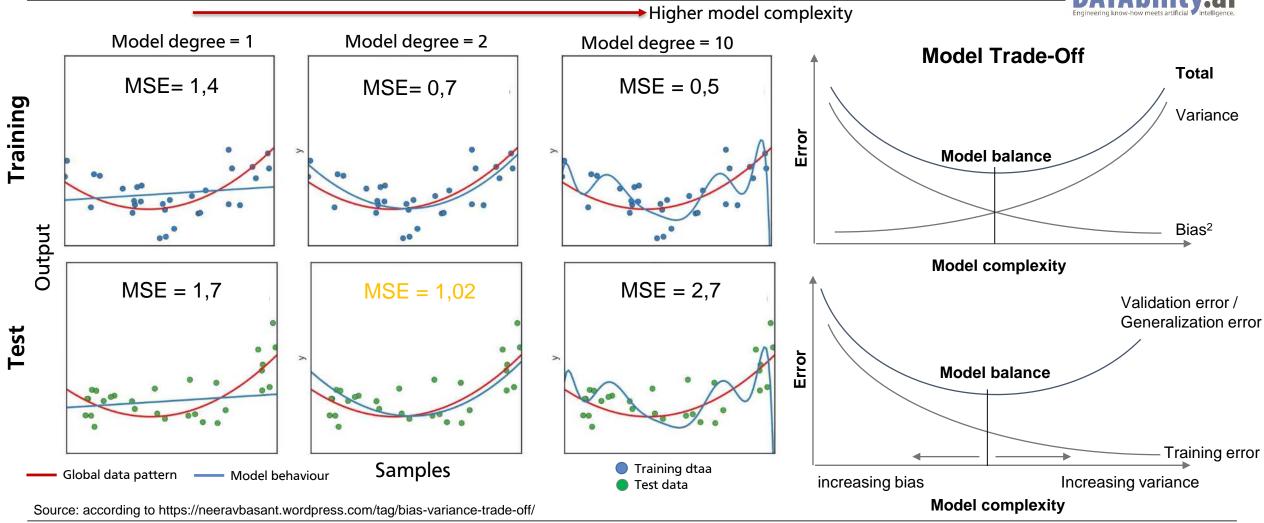


Source: according to https://wp.stolaf.edu/it/gis-precision-accuracy/



Achievement of generalizability





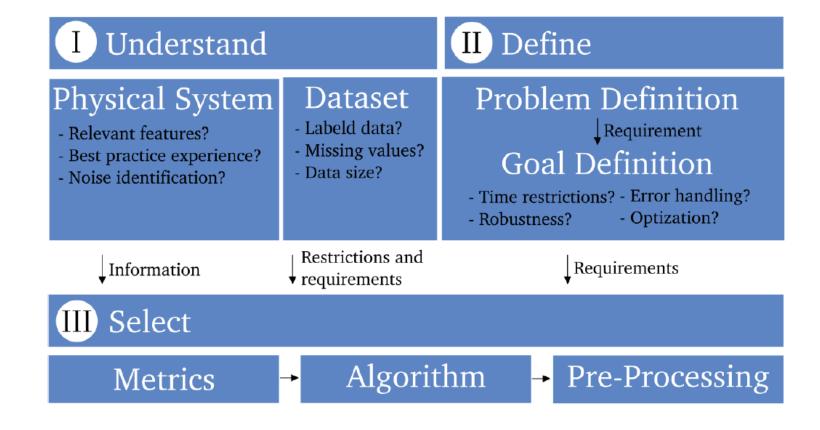


DATA UNDERSTANDING



Suggestion for an approach to select algorithms and strategies







Statistical data understanding and analysis techniques



Descriptive statistics



Explorative statistics



Inductive statistics

Characterisation of the data through metrics and graphics

Search for anomalies in the data and development of hypotheses

Examples:

- Locational and variance metrics
- Graphical methods

Examples:

- Relational metrics
- Graphical methods

Formulation of statements that can be statistically evaluated beyond the data set

Examples:

- Statistical models
- Significance tests



Statistical data understanding and analysis

Methods



Descriptive methods

Locational metrics

- Arithmetic mean
- Median
- Mode
- Quantile
- Minimum, maximum

Variance metrics

- Empirical variance
- Empirical standard deviation
- Mean absolut deviation
- Range
- Inter-quartil-distance
- Variation coefficient

Graphical methods

- Frequency table
- Frequency distribution
- Histogram
- Empirical distribution function

Explorative methods

Graphical methods

- Boxplot
- Q-Q-Plot
- P-P-Plot
- Violinplots
- Scatterplot
- Covariance
- Covariance coefficients

Correlation analysis

- Bravais and Pearson
- Fechner
- Spearman
- Kendall





DATA UNDERSTANDING





EXAMPLE



Example: Statistical Data Understanding

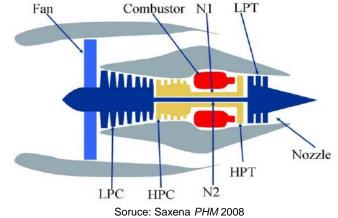
Dataset provided by NASA (CMAPSS – turbofan simulation)

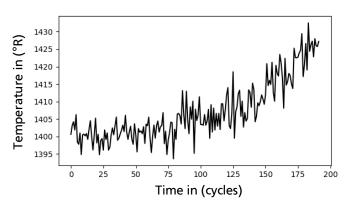


- Task:
 - Diagnosis of health index (HI)
 - Prognosis of the rest of useful lifetime (RUL)

Variables:

- 3 operational settings
- 21 sensor variables
- Artificial noise overlain
- Some features/targets are not directly measurable -> HI indicator
- data processing to eliminate or at least attenuate unwanted signal components





Dataset available for free under:

https://ti.arc.nasa.gov/tech/dash/groups/pcoe/prognostic-data-repository/

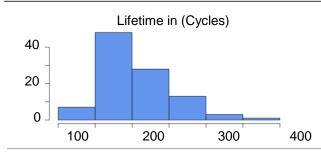


Example: Statistical Data Understanding

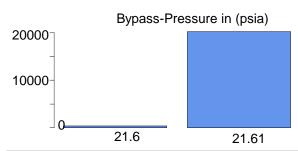
Descriptive statistics



Explorative statistics

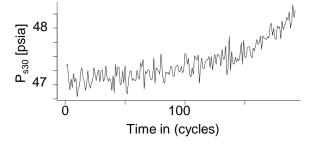


- Average Lifetime: 205 cycles (standard deviation 46,3)
- Range: 127 361



10 variables without relation to health status;

- constant, or discrete characteristics
- only varying through sensor noise



- Different locational and variance metrics at the beginning and end of operations
- Characteristic trend over time

> 12 variables with consistent trend over time suitable for RUL prognosis

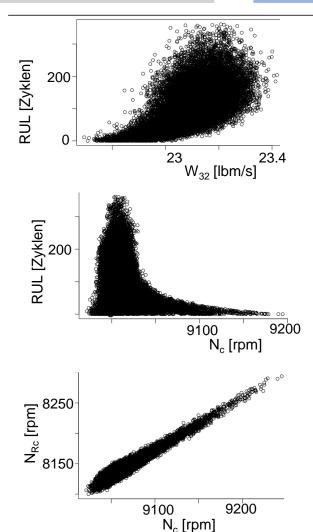


Example: Statistical Data Understanding

Descriptive statistics



Explorative statistics



Correlation analysis:

Varying correlations with RUL

- low importance of the operational variables
- medium correlation for the majority of the sensors
- low correlations for sensors which are constant or show inconsitent trend

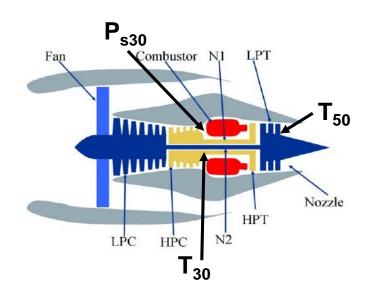
Partly high correlations underneath the sensors \rightarrow redundancies

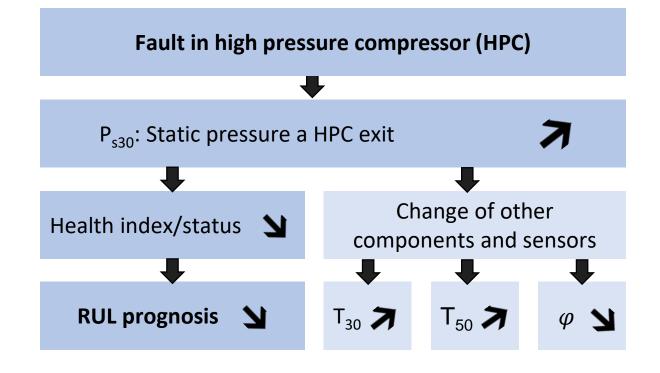
- Different importance and relevance for prognosis
- Potential of feature reduction through dependences



Physical interpretation (based on statistical analysis)











Correlations can help to evaluate redundancies.

However, interpretations may differ from physical insights.

CORRELATION

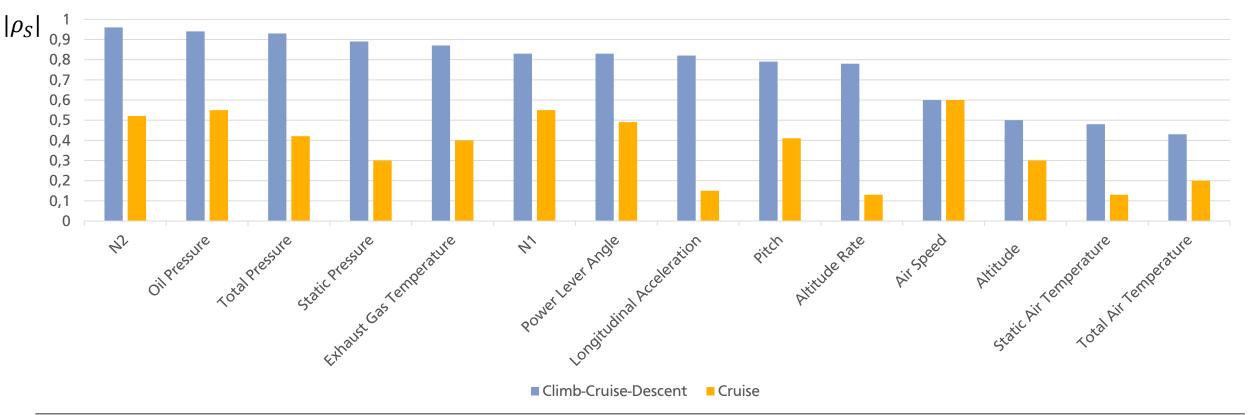


Correlations with the fuel flow of an aircraft in different flight phases.



SPEARMAN correlation coefficient: (Testing for monotony)

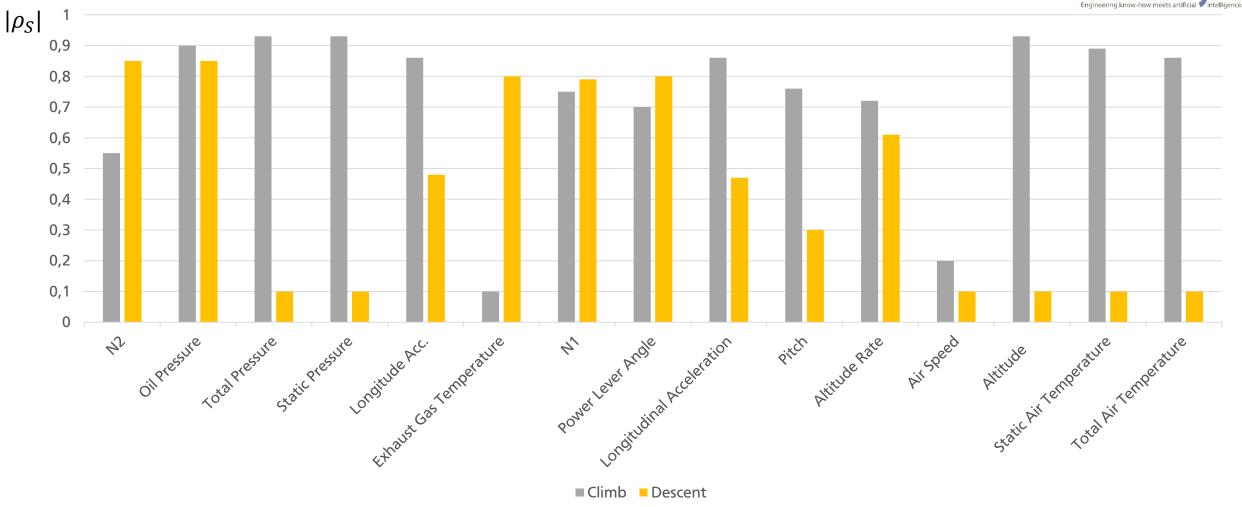
$$\rho_s = \frac{\text{cov}(\text{rg}_X, \text{rg}_Y)}{\sigma_X \cdot \sigma_Y}$$





Correlations with the fuel flow of an aircraft in different flight phases.







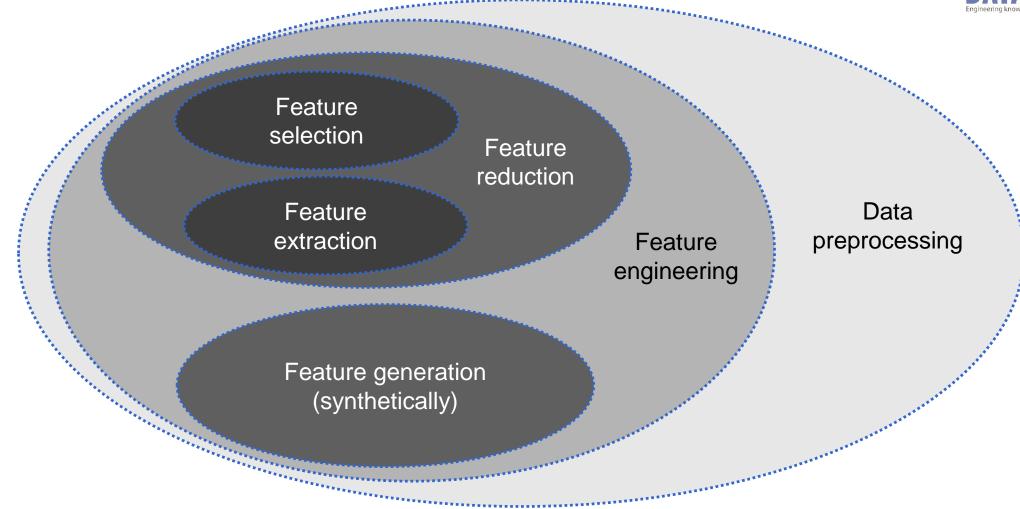


DATA PREPROCESSING: FEATURE ENGINEERING



Classification of feature engineering

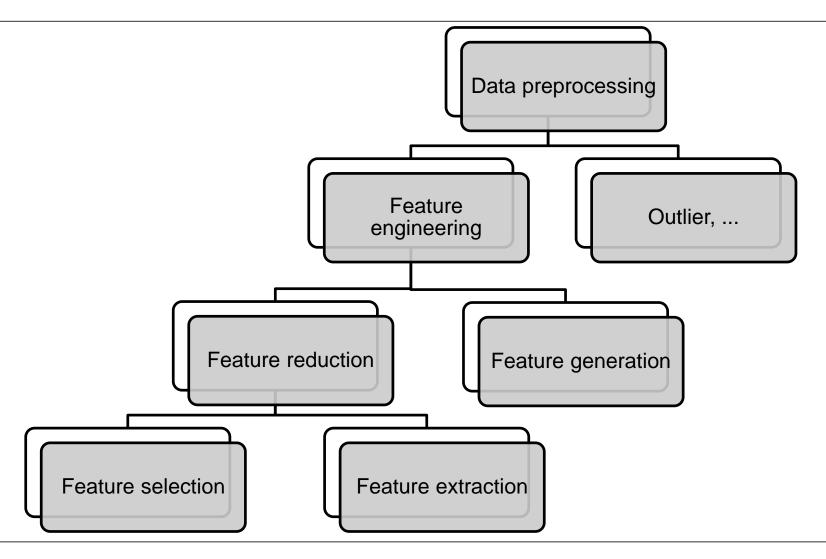






Dependencies in feature engineering







Feature reduction can be devided into feature extraction and feature selection



- Avoidance of multi collinearities and rudundant parameters
- Better generalizability
- Evalutaion of reduction methods through model performance/quality



Feature reduction

Feature extraction

- Principal component analysis (PCA)
- Factor analysis

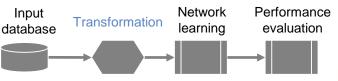


Feature selection

- Wrapper
- Filter
- Embedded



Feature Extraction PCA – Principal Component Analysis





Definition: Source: Jolliffe I.T. Principal Component Analysis (1986)

For a set of *d*-dimensional vectors $\{\mathbf{t}_n\}$, $n \in \{1 ... N\}$, the q principal axes \mathbf{w}_j , $j \in \{1 ... q\}$, are those orthonormal axes onto which the retained variance under projection is maximal.

The eigenvectors \mathbf{w}_j are given by the q dominant eigenvectors of the sample covariance matrix $\mathbf{S} = \sum_{\mathbf{n}} (\mathbf{t}_n - \bar{\mathbf{t}}) (\mathbf{t}_n - \bar{\mathbf{t}})^T / N$ such that $\mathbf{S} \mathbf{w}_j = \lambda_j \mathbf{w}_j$ and where $\bar{\mathbf{t}}$ is the sample mean. The vector $\mathbf{x}_n = \mathbf{W}^T(\mathbf{t}_n - \bar{\mathbf{t}})$, where $\mathbf{W} = (\mathbf{w}_1, \mathbf{w}_2, ..., \mathbf{w}_q)$, is thus a q-dimensional reduced representation of the observed vector \mathbf{t}_n .

Summary

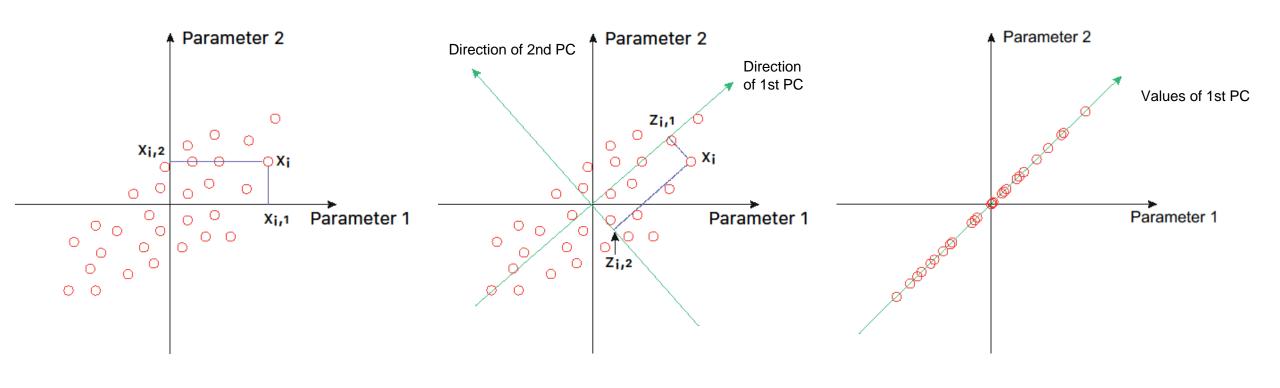
- PCA is an orthogonal linear transformation into a new coordinate system representing the maximum variance
- It is a popular tool for dimensionalty reduction
- The first principal component explains the greatest variance
- The relevance of individual features within a principal component can be interpreted from transformation matrix
- Purpose: explorative data analysis for correlation discovering; modeling with the transformed data can eliminate irrelevant information such as noise and the risk of artifacts such as outliers

Source: http://www.analytik.ethz.ch/vorlesungen/chemometrie/2_PCA_Monitor.pdf



PCA – Visual explanation (Two dimensional)





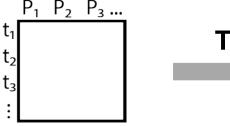


PCA / Factor Analysis – Visual explanation

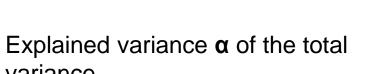


Original data set

variance

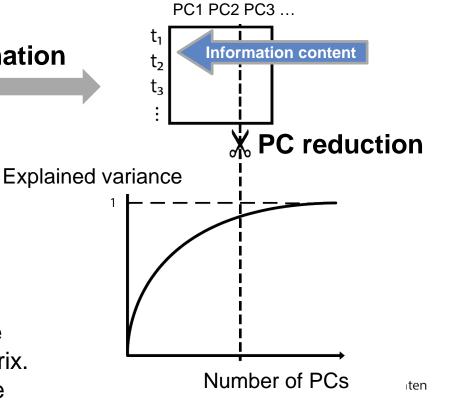


Transformation



Alternative: Kaiser-criterion Determine the eigenvalues of the PCs from the transformation matrix. Eigenvalues greater than one are taken into account for feature (PC) selection.

PC data set



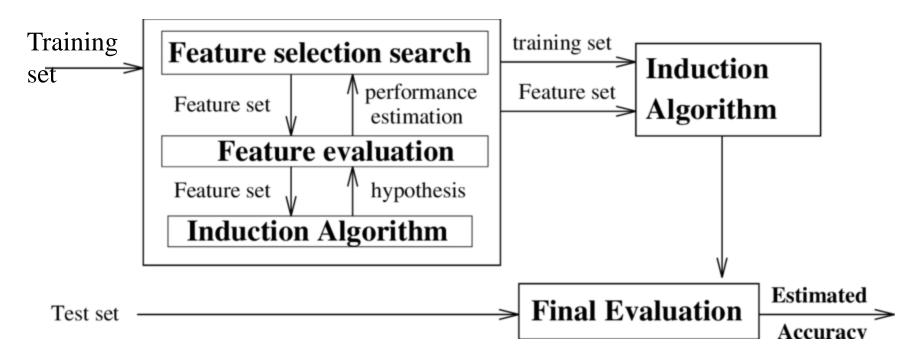
Reduction:

- find a feature set that describes most of the variance while using a fewer number of features
- The obtained latent variables (PC) describe the variance of the data in decreasing order
- The first PC describes most of the variance.
- In order to decide how many PCs are enough to describe the data characteristics, a threshold between 70% to 90% of the described variance needs to be reached by the PCs



Feature Selection approach

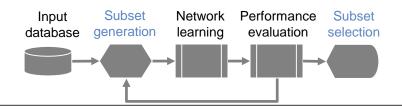




Source: Ron Kohavi: Wrappers for Performance Enhancement and Oblivious Decision Graphs. Stanford University (2015)

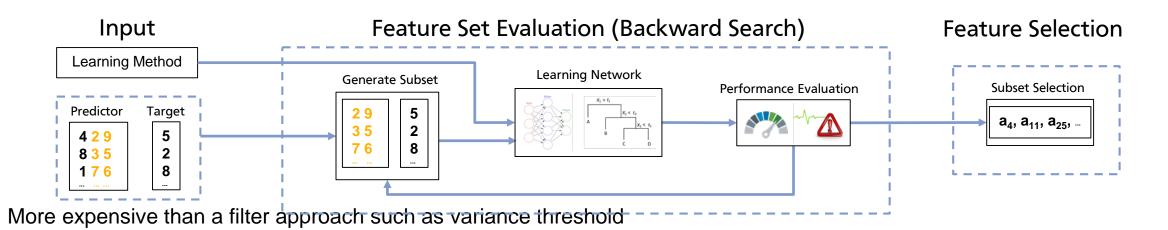


Wrapper using measures for data characterization to select features.



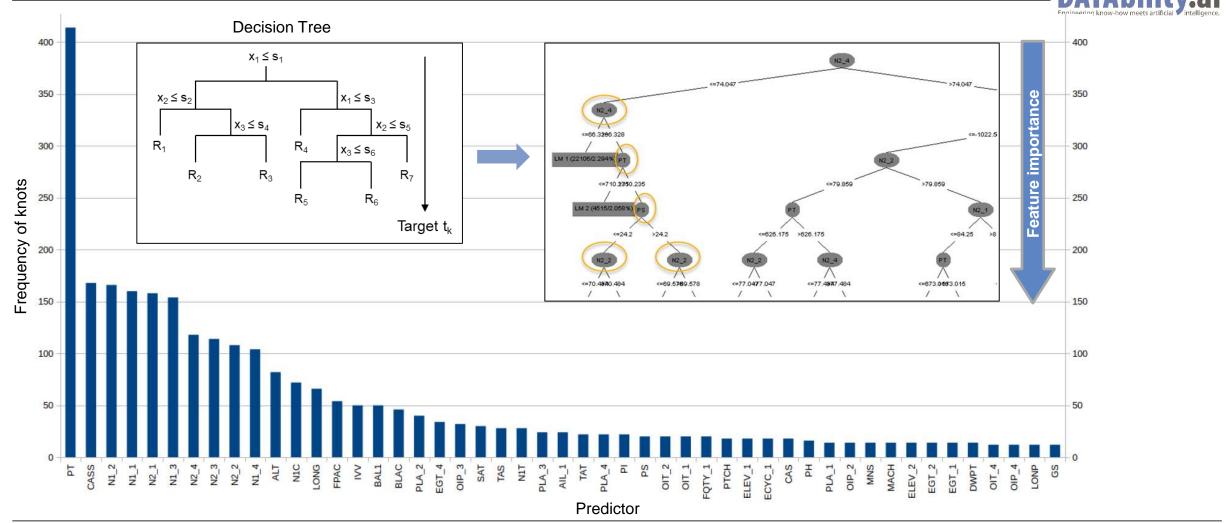


- Forward Search starts with an empty feature subset. The algorithm tries to add every possible attribute to its set and evaluates changes with some performance estimate and, thus, the optimal attribute will be added. The algorithm has also a parameter that allows to make some suboptimal steps, when no attributes can be added with a positive estimation. This is done with back-propagation, therefore if there are no positive tendencies further, last most optimal feature subset is recovered.
- Backward Search starts with a subset of all possible attributes included. Algorithm tries to remove some of them and evaluates the
 results iteratively.





Embedded: Importance of individual predictors for machine learning models via decision trees.







Data Acquisition | Data Understanding | Data Preprocessing

APPLICATION: HANDLING DEVICE (see Lecture 1)



Setup of Automatic Handling Device





- 4-DoF robotic arm that moves boxes
- No integrated sensors → no process information
- → Does the robotic arm move a heavy or a light container?
- Custom retrofit of robotic arm
- Low-cost sensor and microcontroller (~20 €)
- Raw data send via Wi-Fi
- → Automatic data-driven classification in MATLAB

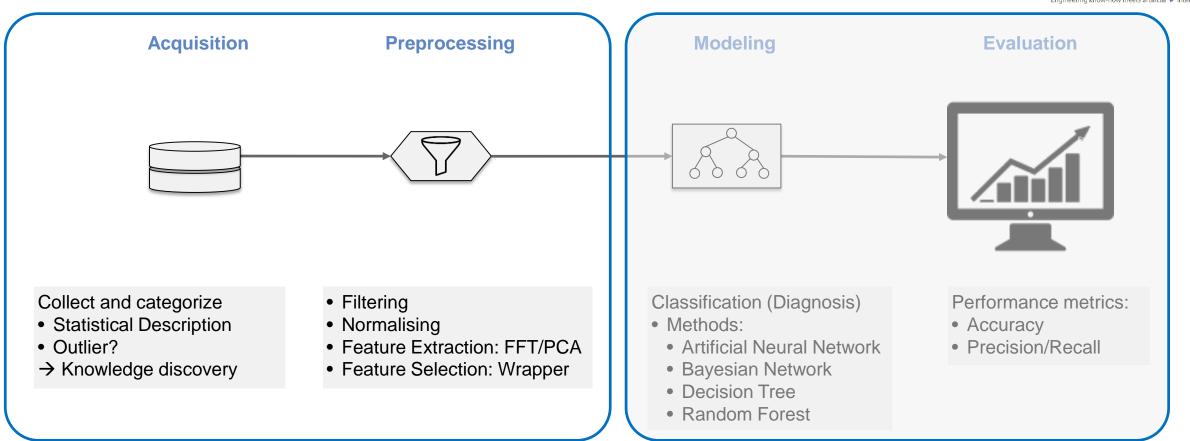


MPU-9250
3-axis Gyro
3-axis Accelerometer
3-axis Magnetometer



Application Framework







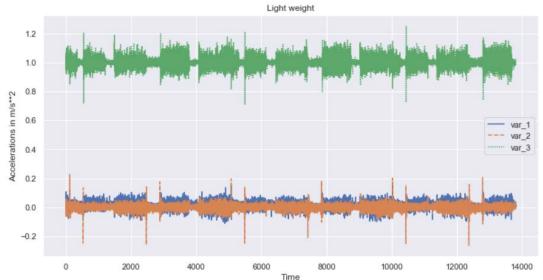
Results: Data Understanding

Descriptive statistics

df light full.describe()

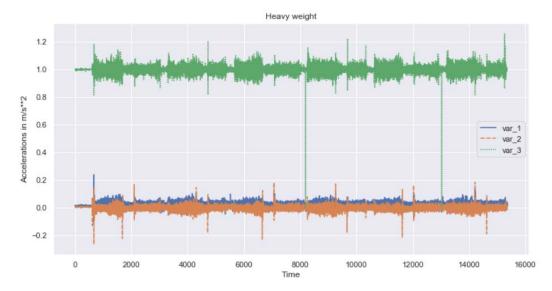


-				
	t	var_1	var_2	var_3
count	13806.000000	13806.000000	13806.000000	13806.000000
mean	400889.231711	0.013772	0.000039	0.999970
std	39877.035927	0.025820	0.024085	0.041814
min	331765.000000	-0.112000	-0.264000	0.708000
25%	366364.500000	-0.000000	-0.012000	0.976000
50%	400897.000000	0.015000	0.001000	0.999000
75%	435409.500000	0.029000	0.013000	1.021000
max	469952.000000	0.154000	0.226000	1.250000



var_3	var_2	var_1	t	
15352.000000	15352.000000	15352.000000	15352.000000	ount
1.000084	-0.001491	0.025510	217449.840607	nean
0.032306	0.020733	0.016597	44658.663301	std
-0.000000	-0.263000	-0.109000	140254.000000	min
0.984000	-0.012000	0.016000	178677.500000	25%
1.000000	-0.000000	0.026000	217437.000000	50%
1.017000	0.009000	0.035000	256122.500000	75%
1.258000	0.186000	0.240000	294706.000000	max

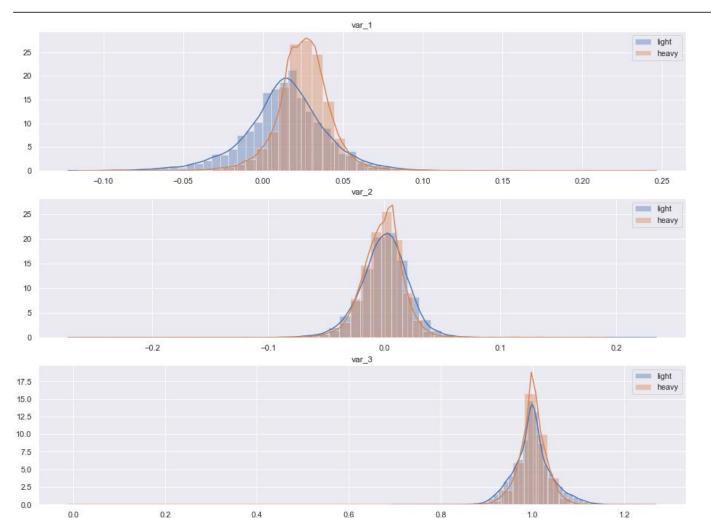
df_heavy_full.describe()





Results: Data Understanding

Explorative statistics

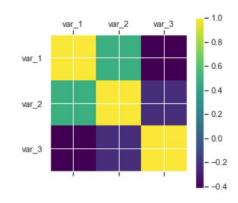


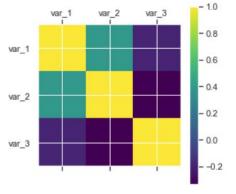


Correlations between accelartions

df_light.corr()			
	var_1	var_2	var_3
var_1	1.000000	0.476959	-0.415627
var_2	0.476959	1.000000	-0.224667
var_3	-0.415627	-0.224667	1.000000

df_heavy.corr()			
	var_1	var_2	var_3
var_1	1.000000	0.381186	-0.194681
var_2	0.381186	1.000000	-0.330959
var_3	-0.194681	-0.330959	1.000000





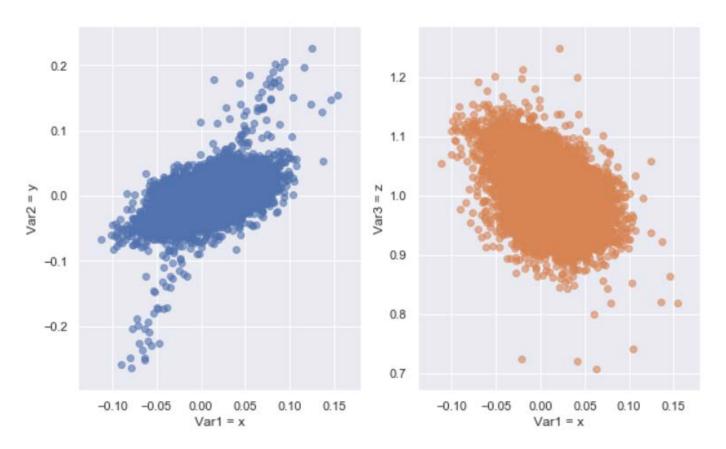


Results: Data Understanding

Explorative statistics



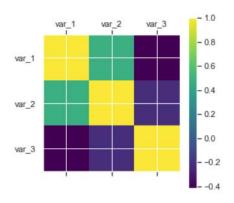
Plotting accelerations against each other

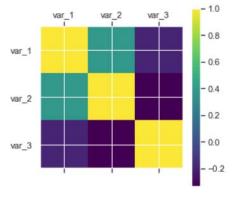


Correlations between accelartions



df_heavy.corr()			
	var_1	var_2	var_3
var_1	1.000000	0.381186	-0.194681
var_2	0.381186	1.000000	-0.330959
var_3	-0.194681	-0.330959	1.000000

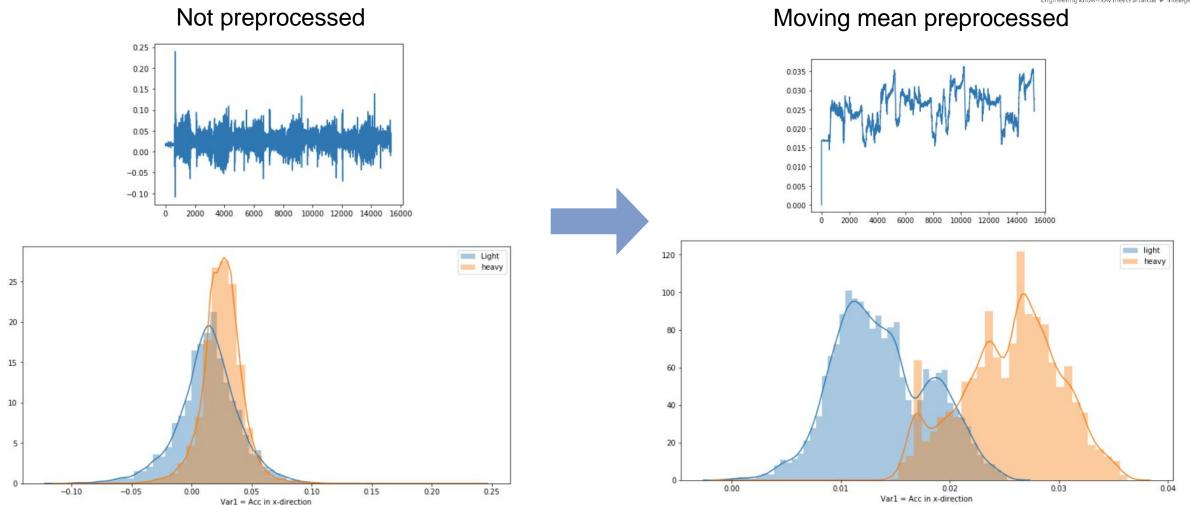






Moving mean (window size = 100)

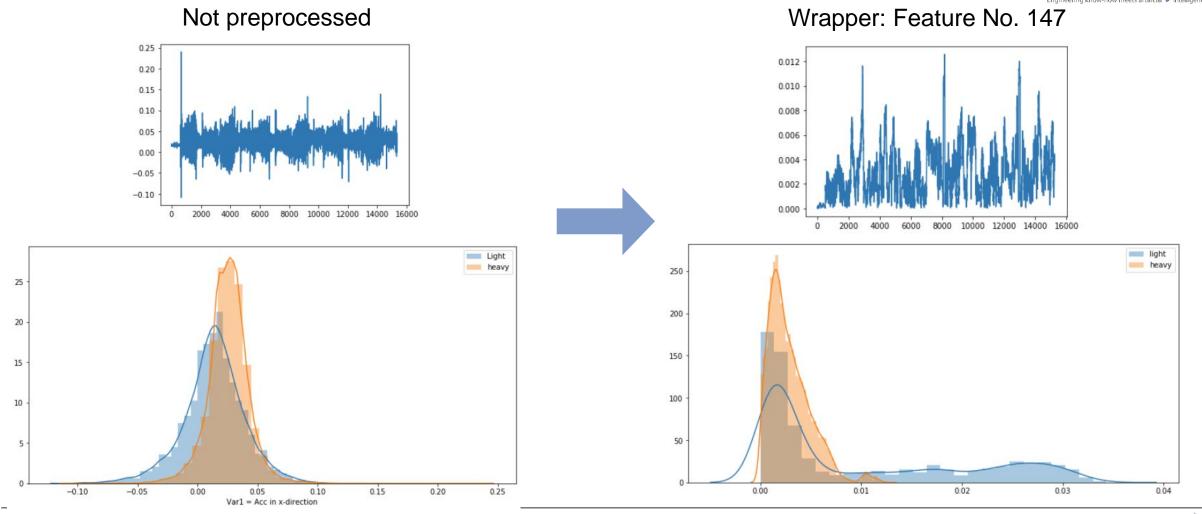






Wrapper based on FFT (150 features!)

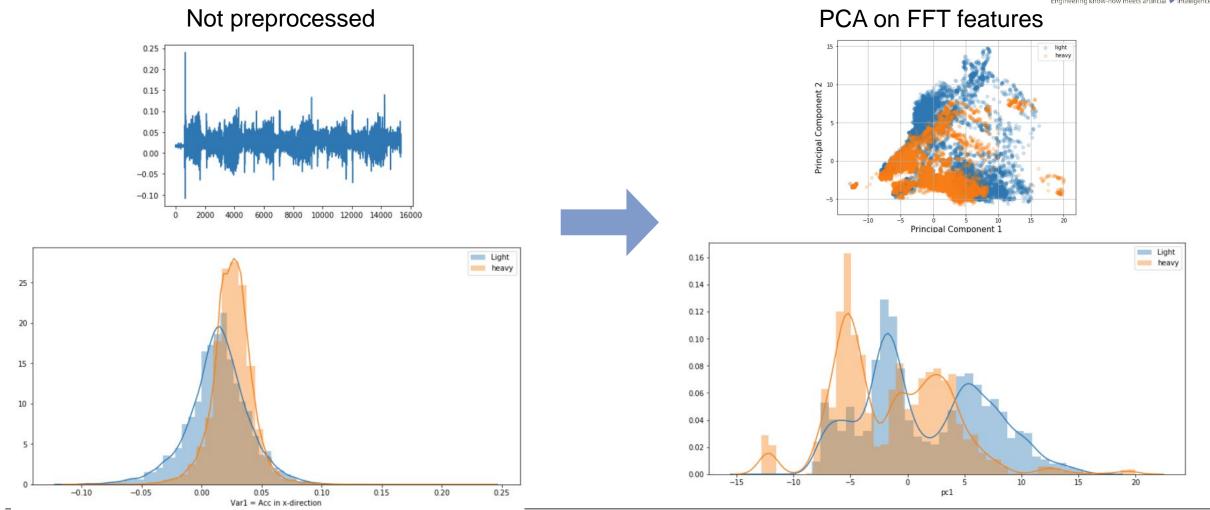






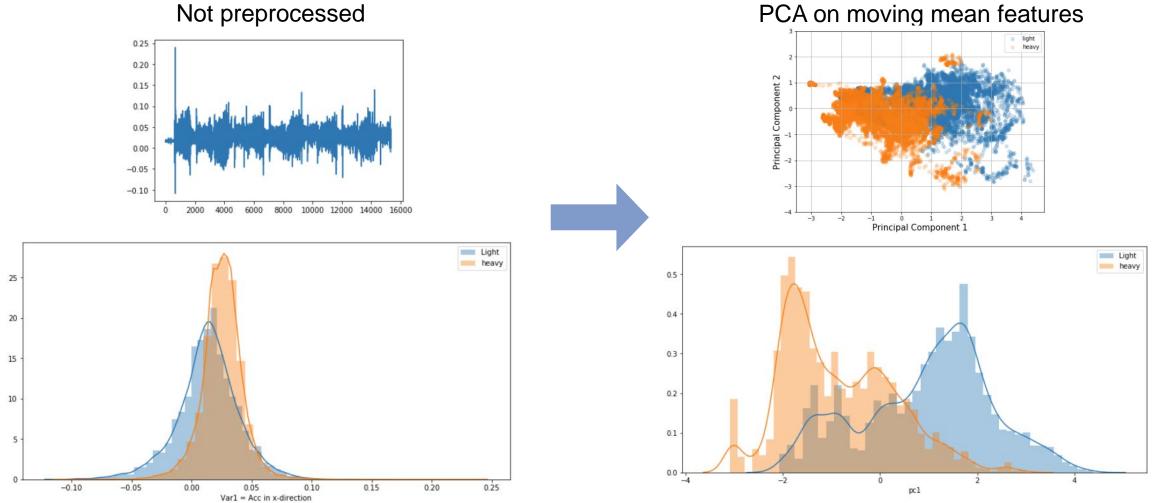
PCA with 3 principle components, based on FFT





PCA with 3 principle components, based on moving mean

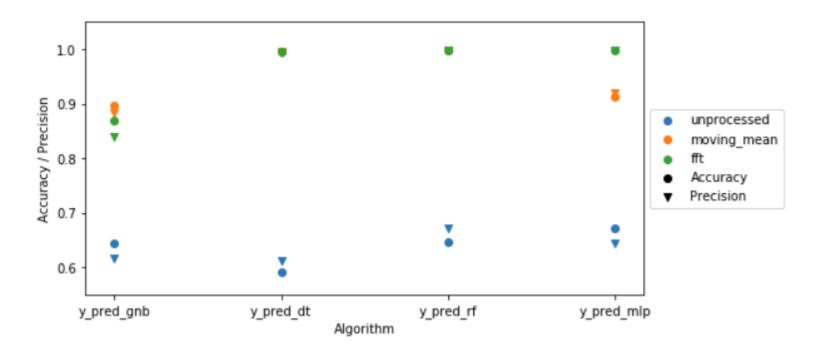




Final results



- Different algorithms
- Different preprocessing methods
- Showing accuracies and precision

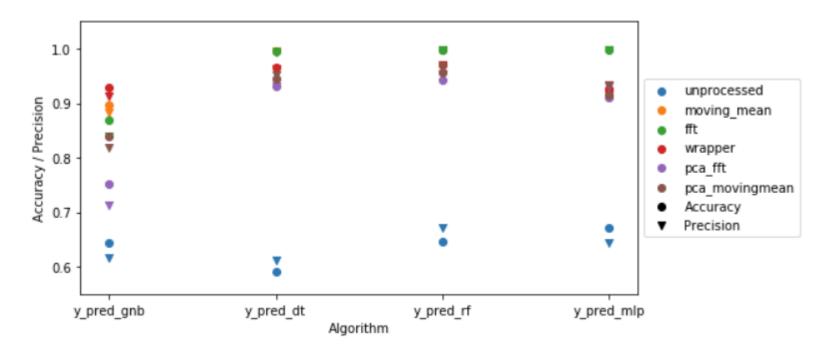




Final results



- Different algorithms
- Different preprocessing methods
- Showing accuracies and precision







What to take with you?

LEARNING OUTCOMES



Key Findings



- Business and data undestanding built the foundation for your model
- Various methods are available for data preprocessing, an appropriate selection depends on many influences, mostly on the analysis question
- Many of them can be combined in creative ways
- Outlier detection is an important step to increase data quality
- Data quality is the key to success prevent garbage in, garbage out
- Feature selection methods are used to focus on meaningful features
- Feature reduction methods reduce model complexity
- Grey box modeling is the key for technical domains, reviews are obligatory



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