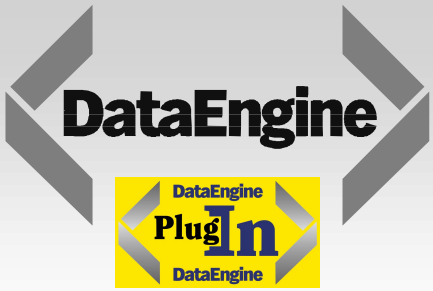
Application of the ProcessAnalyzer in Chemical Industry

Torsten Schrötter



Application of the ProcessAnalyzer in Chemical Industry

- Task
- Realization
- Results of Data Analysis
- Conclusion

Task

- Revealing cause and effect relationships
- Gaining Knowledge from dynamic process data
- Evaluation of ProcessAnalyzer

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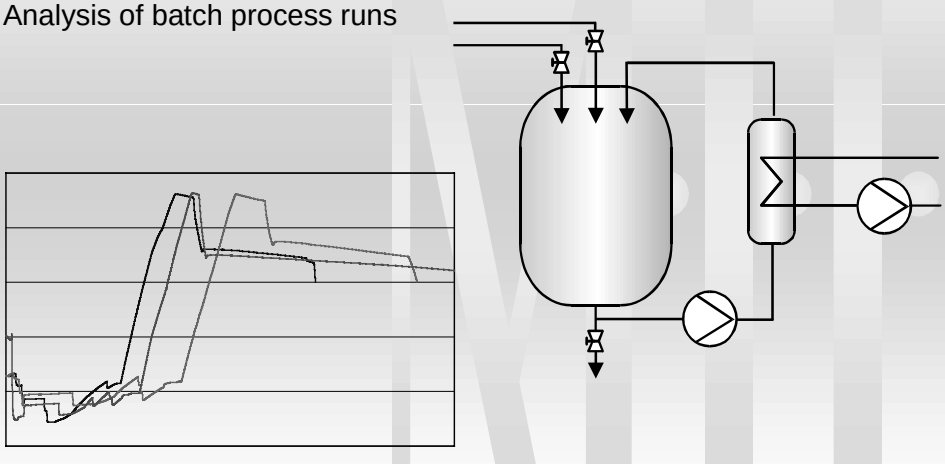
Task

Analysis of batch process runs



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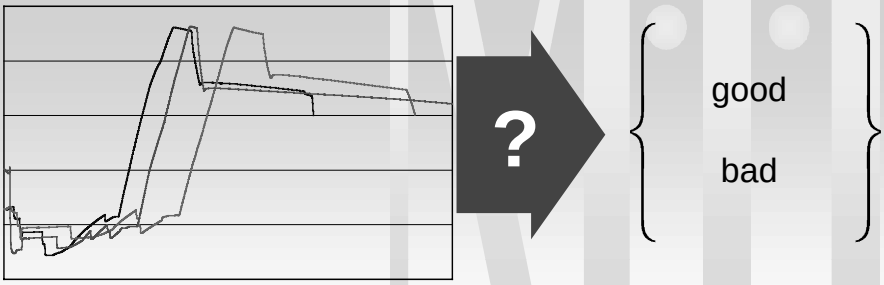
Objective

Modeling of a classifier

- Quality
  - Purity
  - Brightness
  - ...



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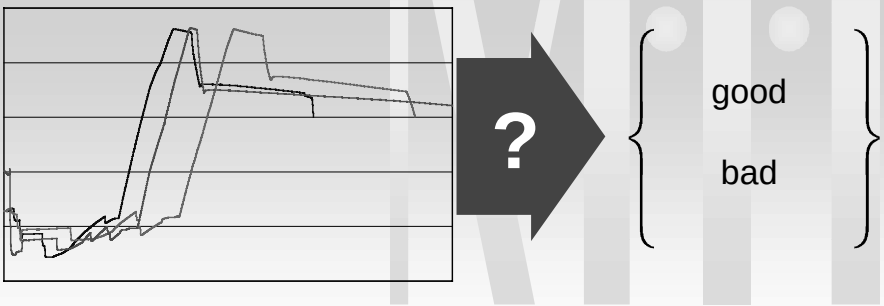
Method for Knowledge Acquisition

- Decision Tree: **DataEngine PlugIn DecisionXpert**



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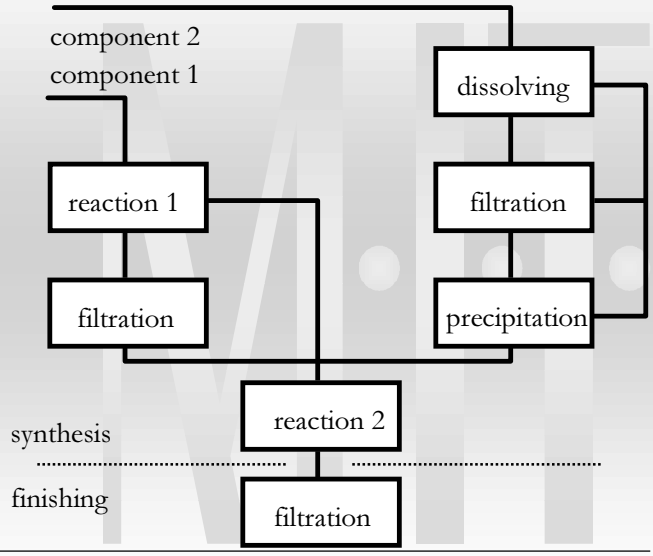
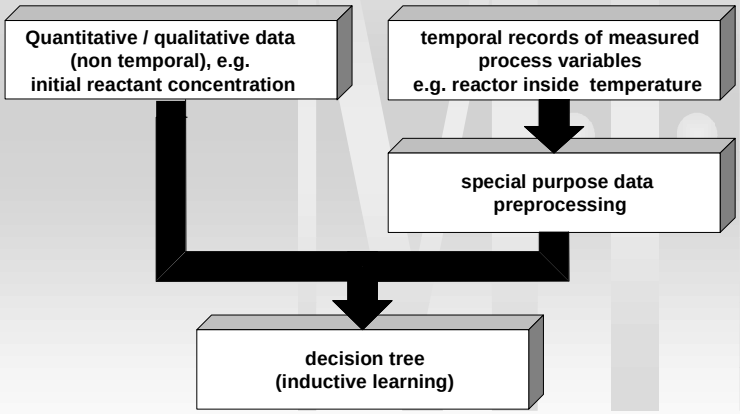
Process
(cutout section)



Realization

- Procedure of Data Analysis
- Data Basis
- Data Preprocessing
- Modeling of Classifiers

Procedure of Data Analysis



Data Basis

- Data source: production of an organic pigment
- 131 batches
- 3 *dynamic process variables*
- 66 static process parameters,

  9 *quality parameters*
- Objective of the analysis: 6 quality parameters

Dynamic Process Variables

- Continuous recording (115 days)

  → splitting of batch data

- measured time series: 5000 samples per batch

Quality parameters

- Brightness, hue, purity
  - ordinal characteristic
  - range [-6; 6]
  - target: [-2; 2]
- Color strength [%] metric
  - target: [100% - Δ; 100% + Δ]
- dH [CIELAB] metric
  - target: [-Δ ; Δ]

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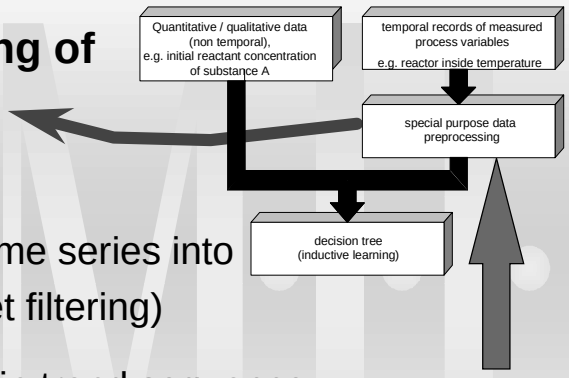
Data Preprocessing of Time Series



- Decomposition of time series into trends (after wavelet filtering)
- Pattern recognition in trend sequence
- Feature generation

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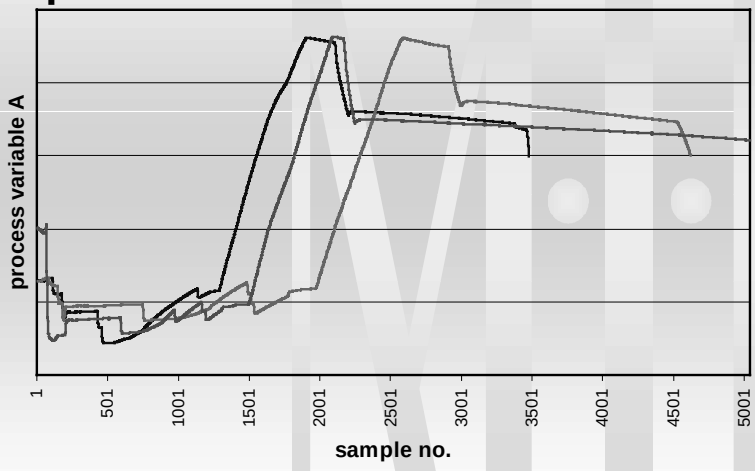
Example



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Wavelet Filtering

- Analysis of transition processes with different dynamics
- Time dependent decomposition into frequency ranges
- Utilization of Cubic Spline Wavelets

→ Analysis with adequate resolution

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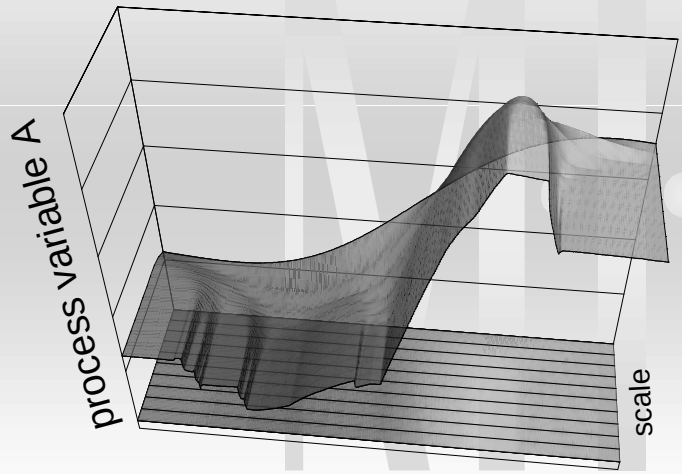
Wavelet Filtering



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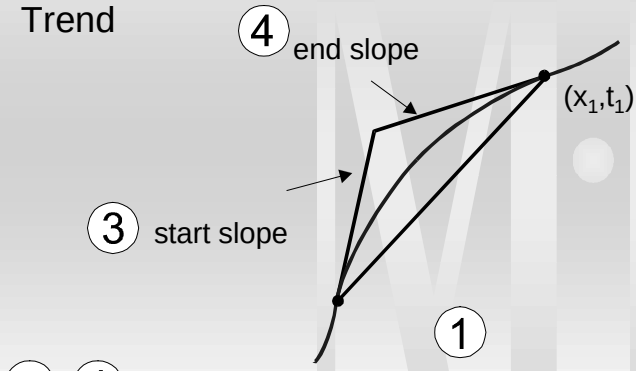
Dekomposition of Time Series

- Trend



measured values,
start and end time
of trend limits
- inflection point
- max / min

1-4 ⇒ quantitative features

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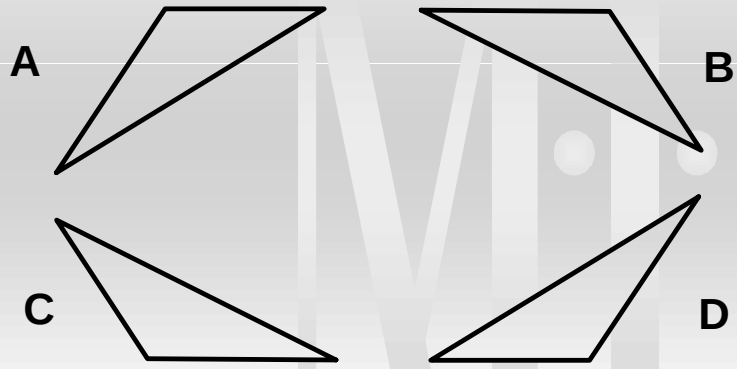
Basic Types of Trends



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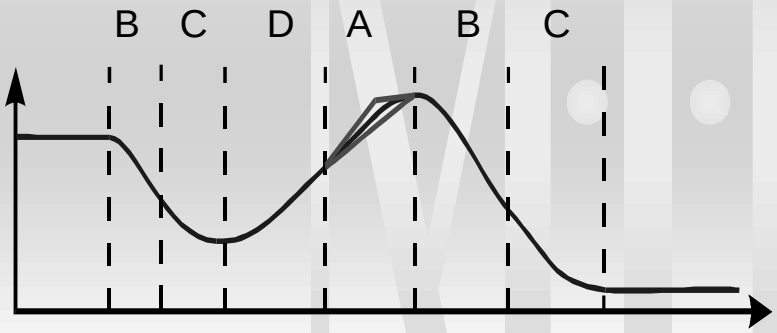
Qualitative Representation of Time Series

"generalized description" = trend decomposition



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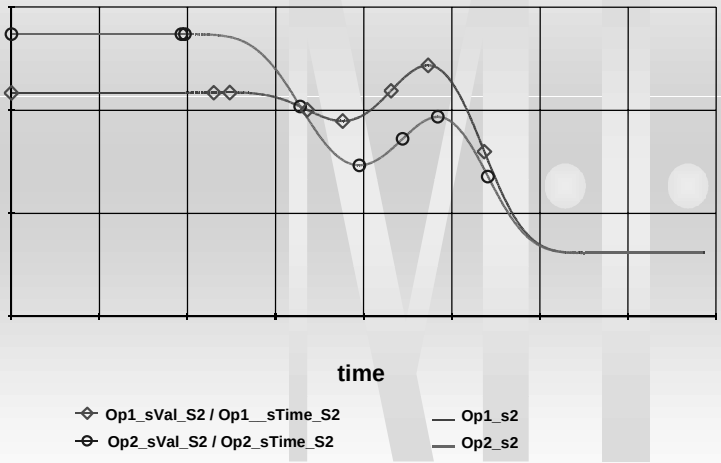
Trend Decomposition



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Pattern Recognition in Trend Sequences

Enables comparison of

- quantitative features
- originating from several process runs

→ Matching of features that represent equivalent events

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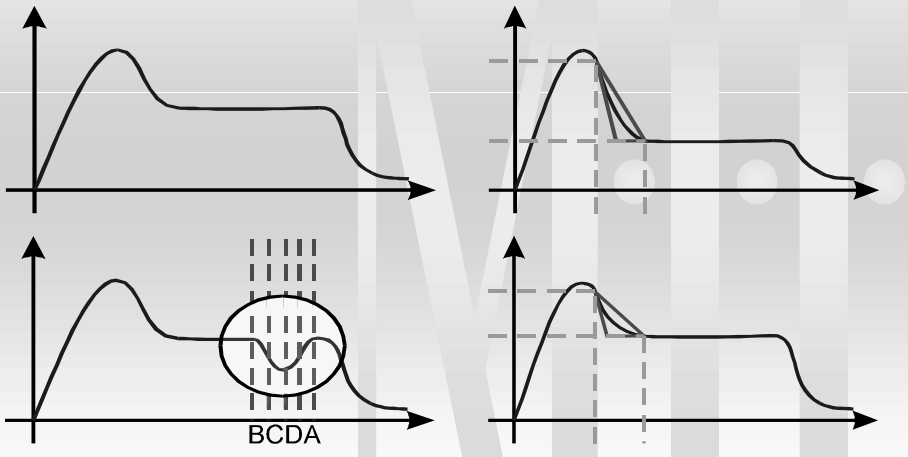
Feature Generation



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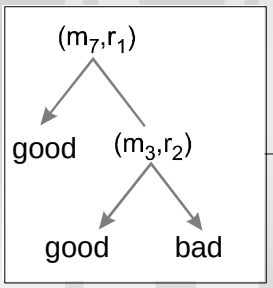
Modeling of Classifiers

- **Available Data**
  Features m_i
  non - temporal
  qualitative → (cardinal/ordinal)
  quantitative → (metric)
  of trends → quantitative



Classification of process output C_i

{ good, bad }

- **Results** set of rules { r_i }

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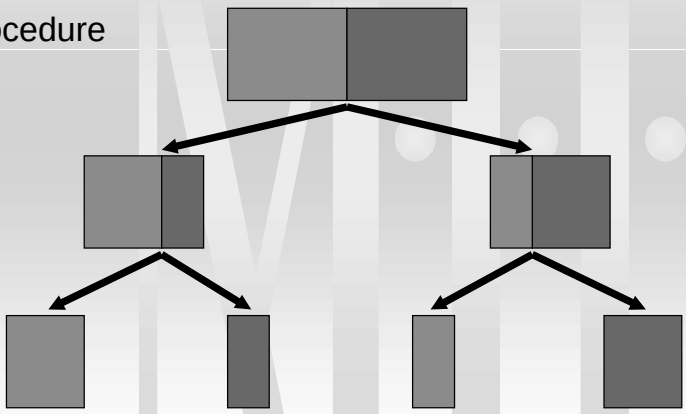
Induction of a Decision Tree

General Procedure



Results of Data Analysis

- Preprocessing of Process Signals
- Classification
- Decision Tree for Quality Parameter

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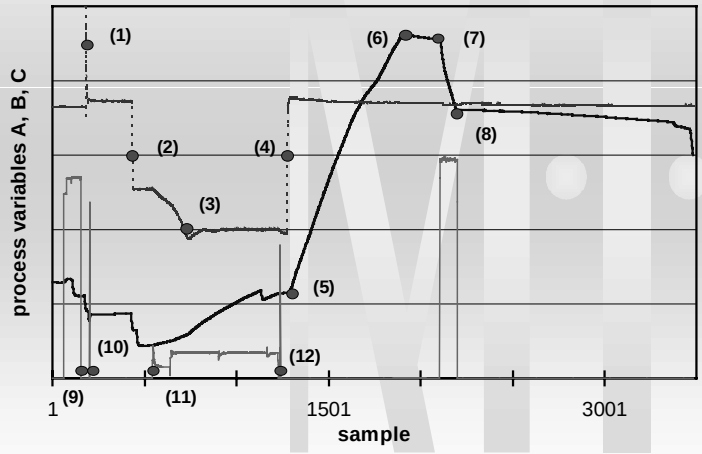
Preprocessing of Process Signals



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Times

- t(1), .., (12)
- Differences of each combination of two times t(1), .., (12)

Process Variable C

- Integral, mean value and variance t(11) – (12)

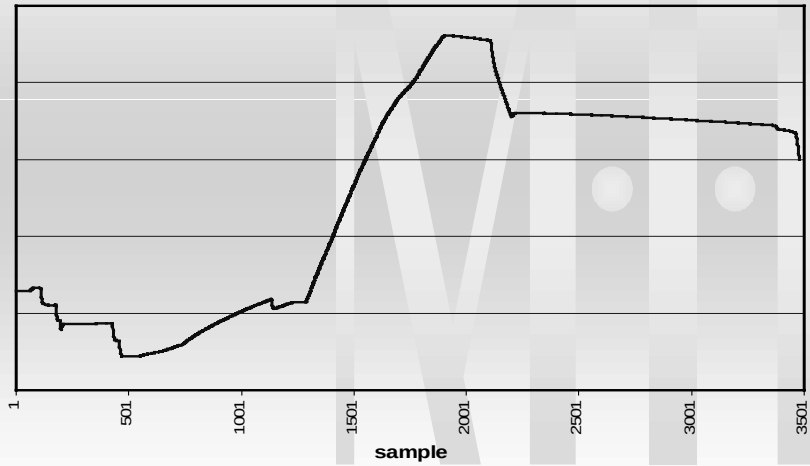
Process Variable B

- Sum of squared deviation from the desired value t(3) - (4)
- Sum of positive differences t(3) - (4)
- Number of samplings with positive differences t(3) - (4)
- Mean value of positive differences (quotient of 2. and 3.)
- Sum of absolute values of negative differences t(3) - (4)
- Number of samplings with negative differences t(3) - (4)
- Mean value of the negative differences (quotient of 2nd and 3rd)

Process Variable A

- Measured values at times t(1), .., t(12)
- Mean gradient, integral, mean value and variance during the sequence from t(11) to t(12)
- Integral and mean value from t(5) to t(8)
- Mean gradient between t(5) - t(6) and t(7) - t(8)

Signal Shape of Process Variable A



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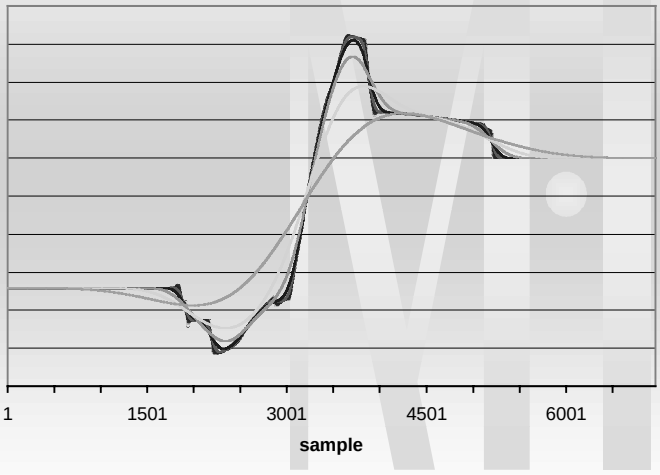
Wavelet Filtering of Process Variable A



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Classification

- Assignment of classes „on target“ and „off target“
  - by visual assessment or
  - by the analysis value of the quality parameter
- Induction of decision trees for different selection measures

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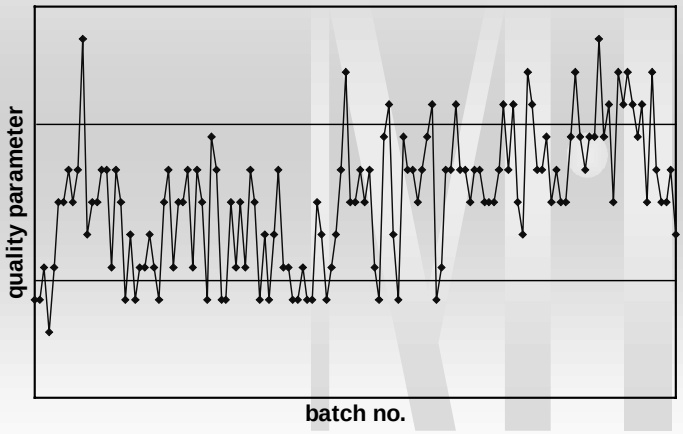
Quality Control Chart



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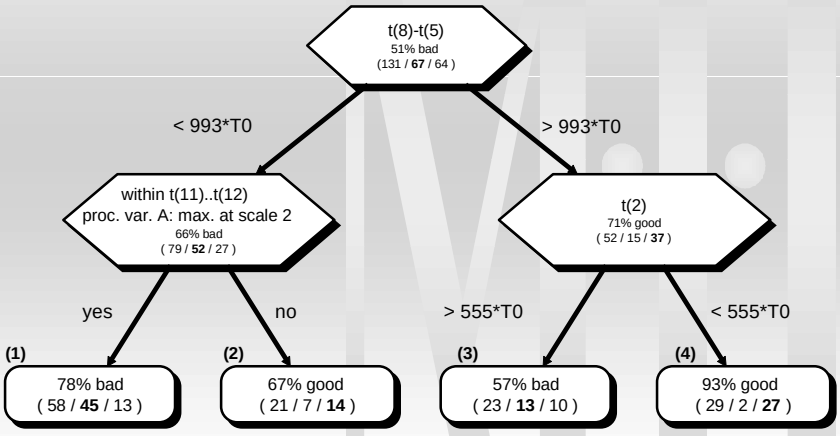
Decision Tree for Quality Parameter



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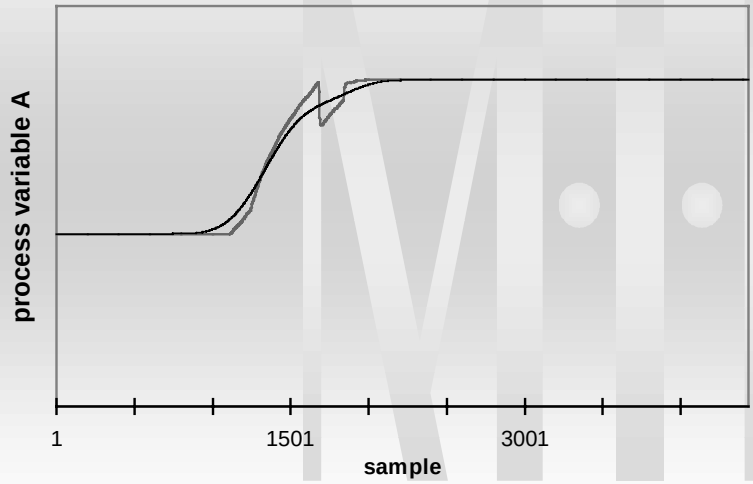
Case 1: Process Signal of Variable A t(2)-(4) at Scale 2



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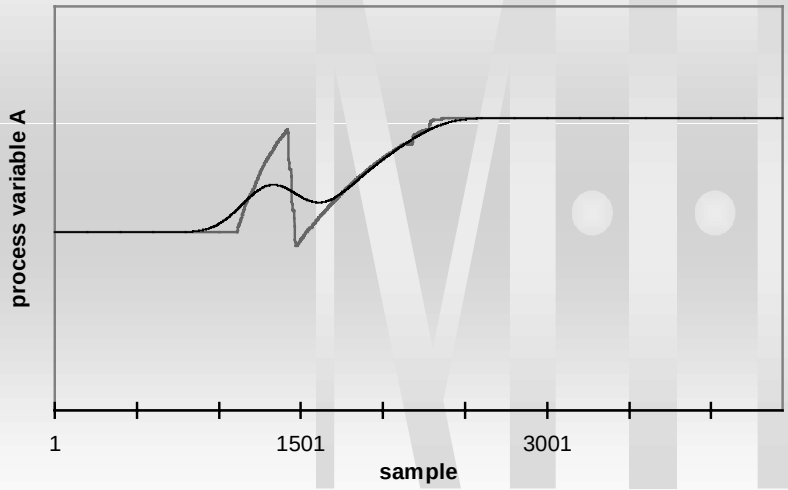
Case 2: Process Signal of Variable A t(2)-(4) at scale 2



Conclusion

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- Consideration of static and dynamic process data
- Rule generation from process data via induction of decision trees
- Information from static data: e.g. influence of (low) values of process variable A on quality
- Information from dynamic data: e.g. influence of process variable A(t(2) - t(4)) on quality (if possible shape without max.)

Conclusion

- Application field: knowledge acquisition (batch processes)
- In this application:

  extracted knowledge ➡ basis for the improvement of
  - Operator instructions
  - Unit recipe
  - Control recipe