# AI in Manufacturing for Process Optimization

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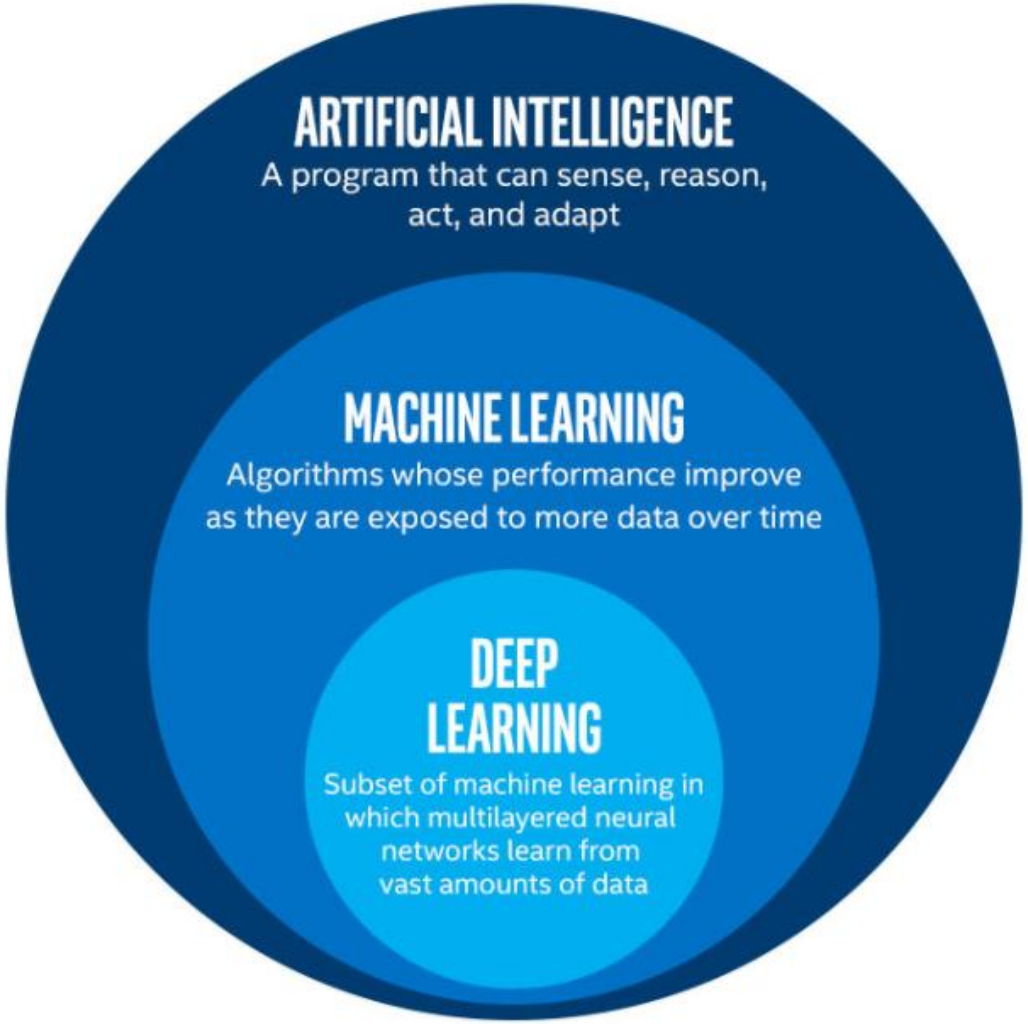
# Overview

- Intro: AI (high level)
- Automated Machine Learning
- Production Process Application Examples
- In vitro Discovery Example
- Concluding

# Foundations

## Artificial Intelligence & Machine Learning

- Algorithms coming as close as possible to human capabilities.
- Includes machine learning→ Learning from data
- „deep learning“ is a subgroup of machine learning

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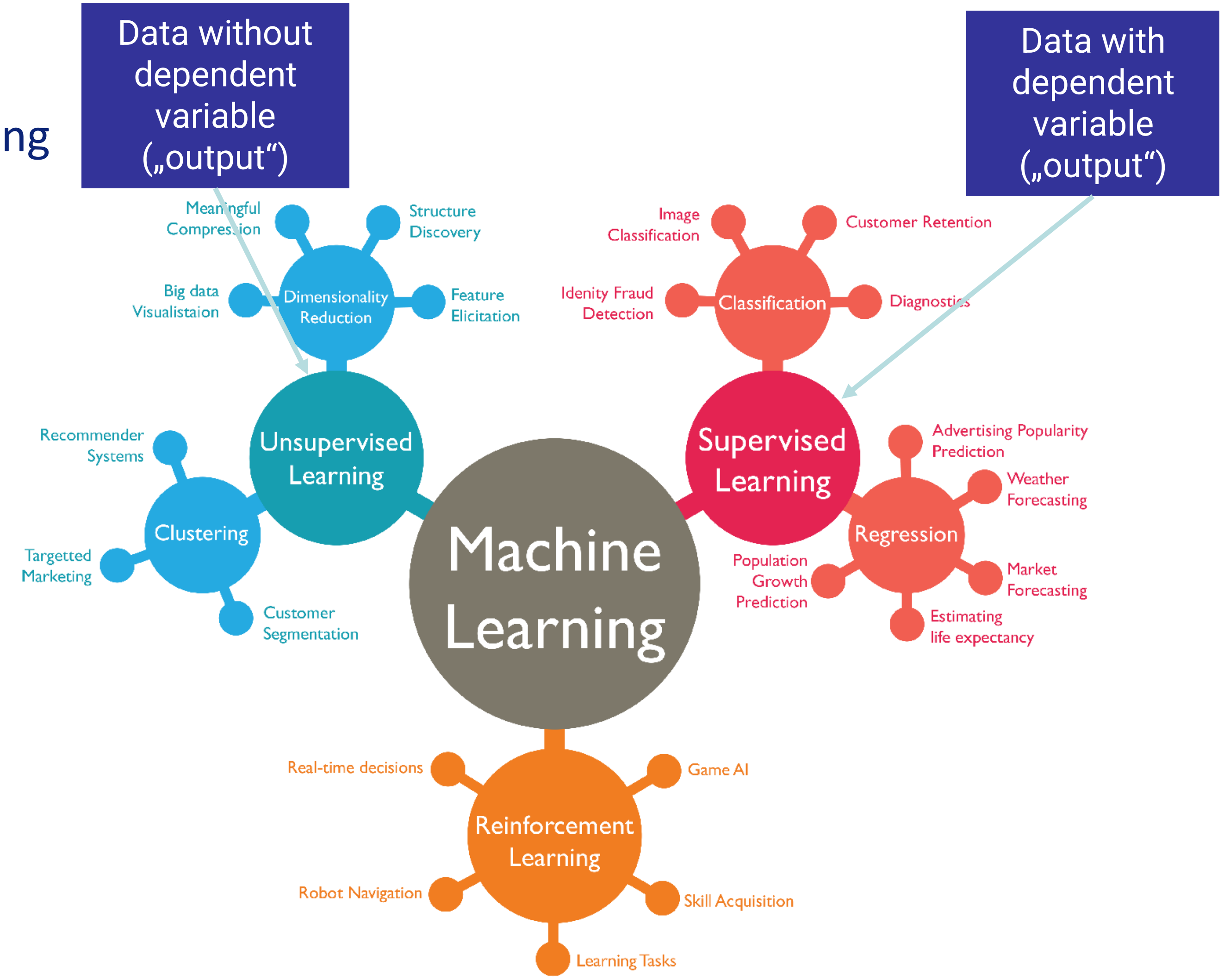
# Foundations

## What is „machine learning“ ?

- Unsupervised – supervised – reinforcement learning
- Automated machine learning
- State-of-the-art methods in AI research

## What else do we need?

- Data preprocessing and cleansing
- Often also feature extraction / engineering
- Optimization methods, also multi-criteria

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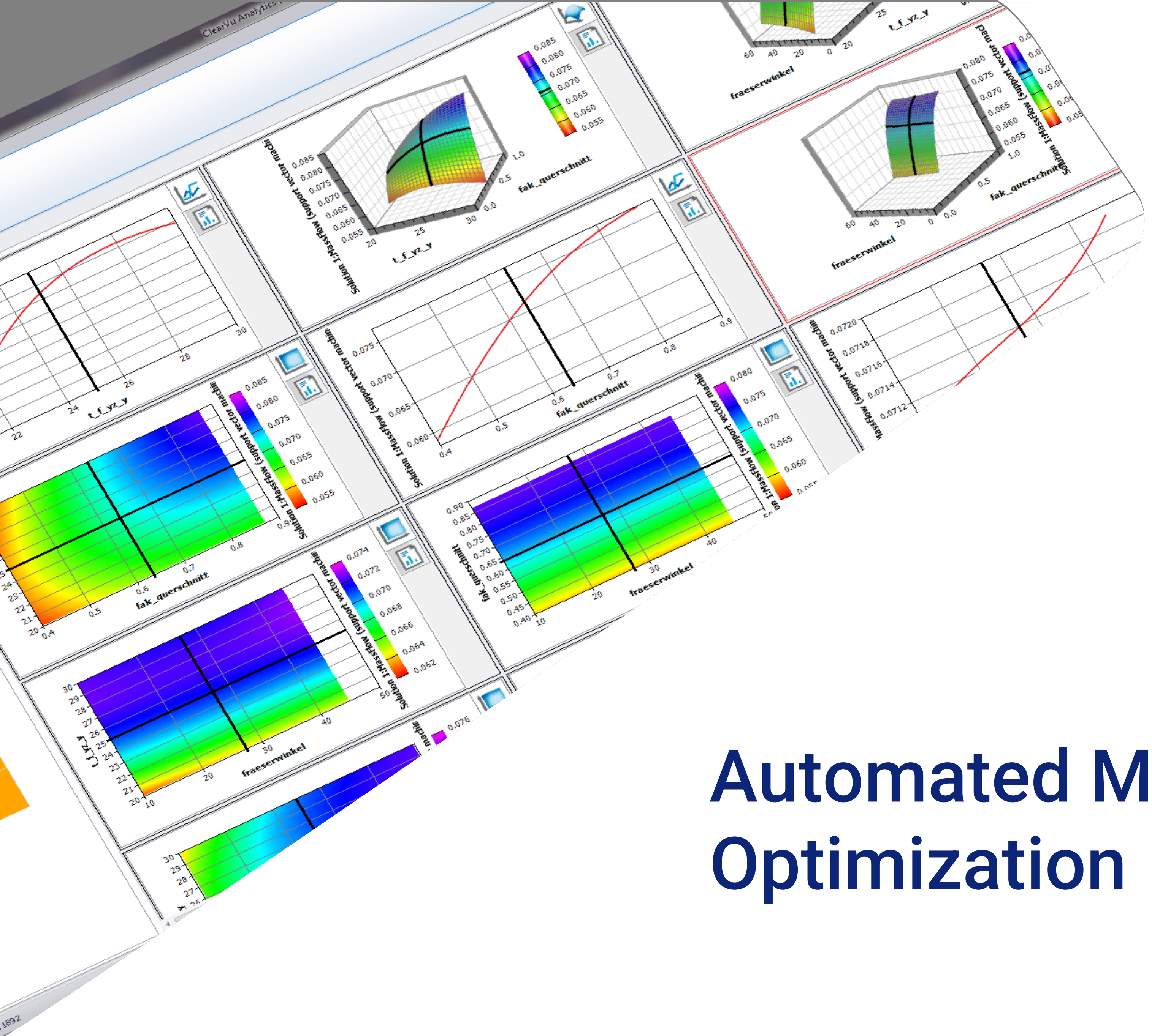
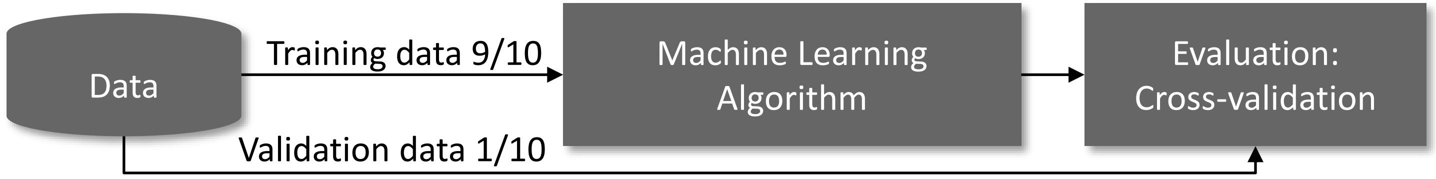



# Automated Machine Learning & Optimization

# Automated Machine Learning

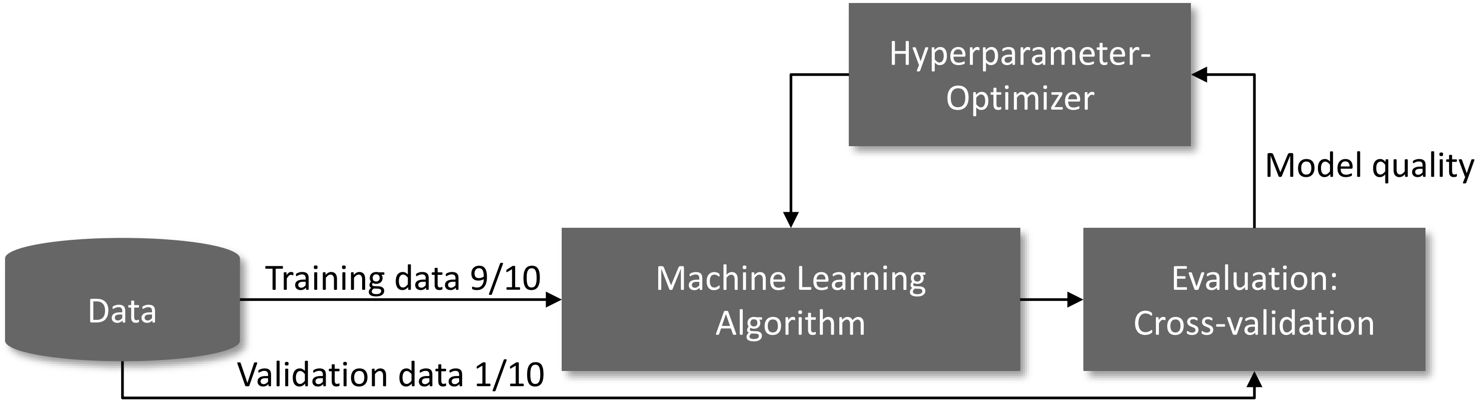
- One algorithm, training and 10-fold cross-validation




- Algorithms: GLM, SVM, Decision Tree, Random Forest, Gaussian processes, partial least squares regression, kernel quantile regression, fuzzy rule sets, feedforward neural network, etc.

# Automated Machine Learning

- One algorithm, hyperparameter optimization, training and 10-fold cross-validation

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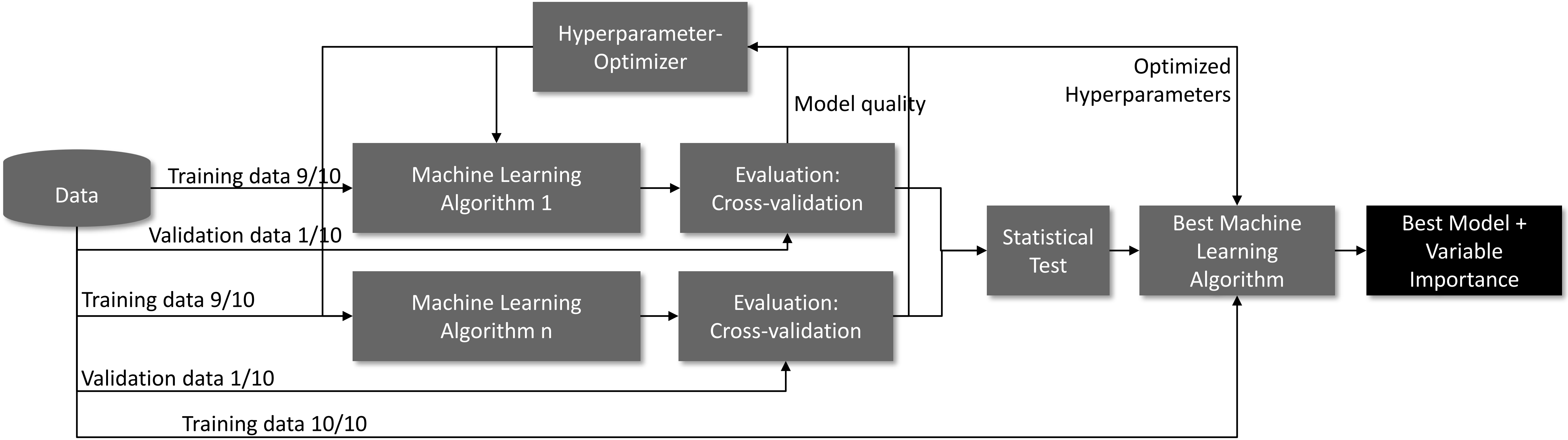
# Automated Machine Learning

- Many algorithms, hyperparameter optimization, training and 10-fold cross-validation, best model selection

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# Automated Machine Learning

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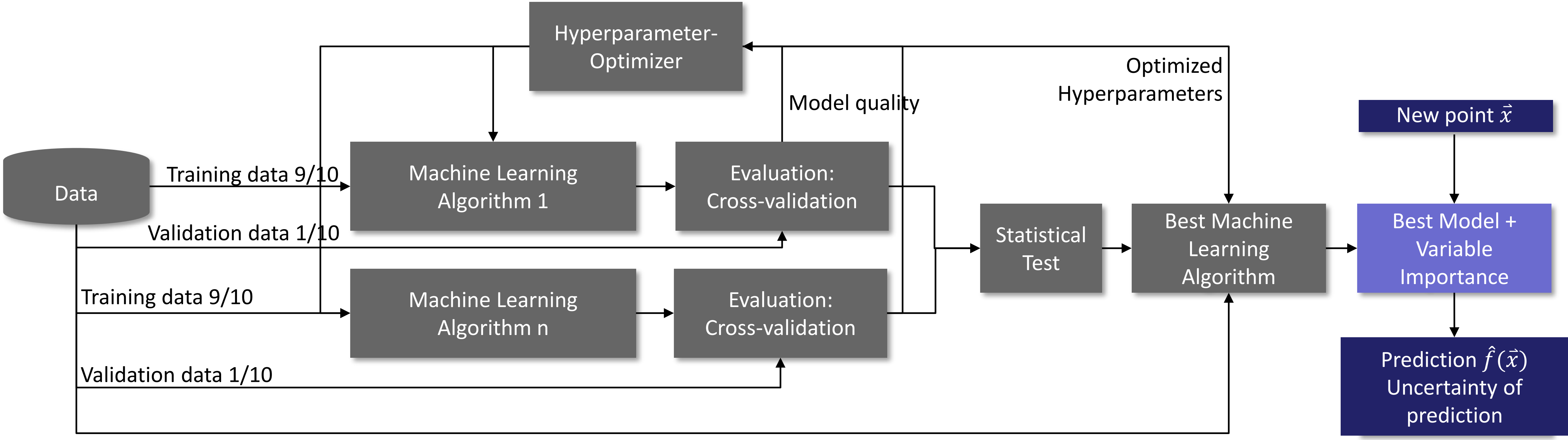



- Algorithms: GLM, SVM, Decision Tree, Random Forest, Gaussian processes, partial least squares regression, kernel quantile regression, fuzzy rule sets, feedforward neural network, etc.


T. Bäck, C. Foussette, P. Krause: *Automatic Metamodeling of CAE Simulation Models*. ATZ Worldwide **117(5)**,36-41, 2015.

X. Guo, B. van Stein, T. Bäck: *A new Approach Towards the Combined Algorithm Selection and Hyperparameter Optimization Problem*. IEEE SSCI, 2042-2049, 2019.

# Example 1:
# Batch Process Optimization

# A Client Example, 2021: Data Analytics for Production

IOI OLEOCHEMICAL

## Thomas Kummer, COO, IOI Oleo GmbH, Witten, Germany

- IOI Challenge: Production of a specialty product for cosmetics industry  caused too many out-of-spec (OOS) batches – which could not be sold
- IOI could not identify the root cause
- Available data:
  - 58 production batches of the product
  - 19 sensor signals, about 3,500 data records per batch

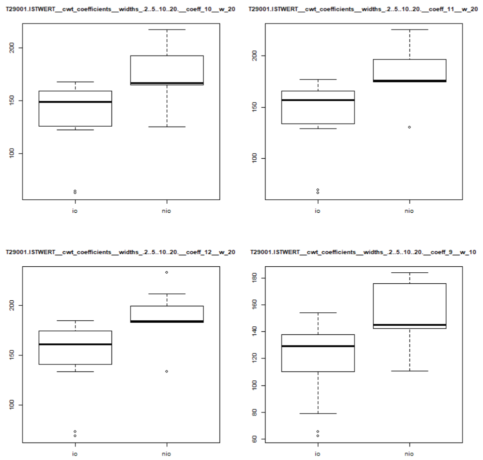
# Technical Approach (Outline)

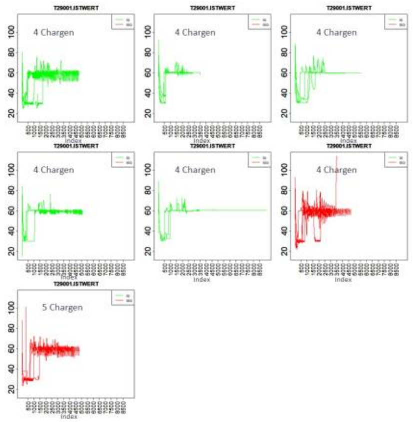
IOI OLEOCHEMICAL

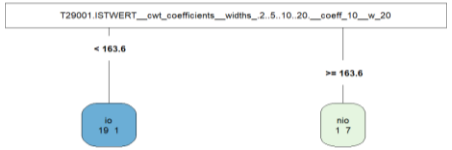
## Data Analytics Steps:

Data preprocessing → Exploratory data analysis → Feature Engineering → Machine Learning → Interpretation and Deployment

batch 000001 batch 000002 batch 000003
...
batch 000025 batch 000026 batch 000027
batch 000028







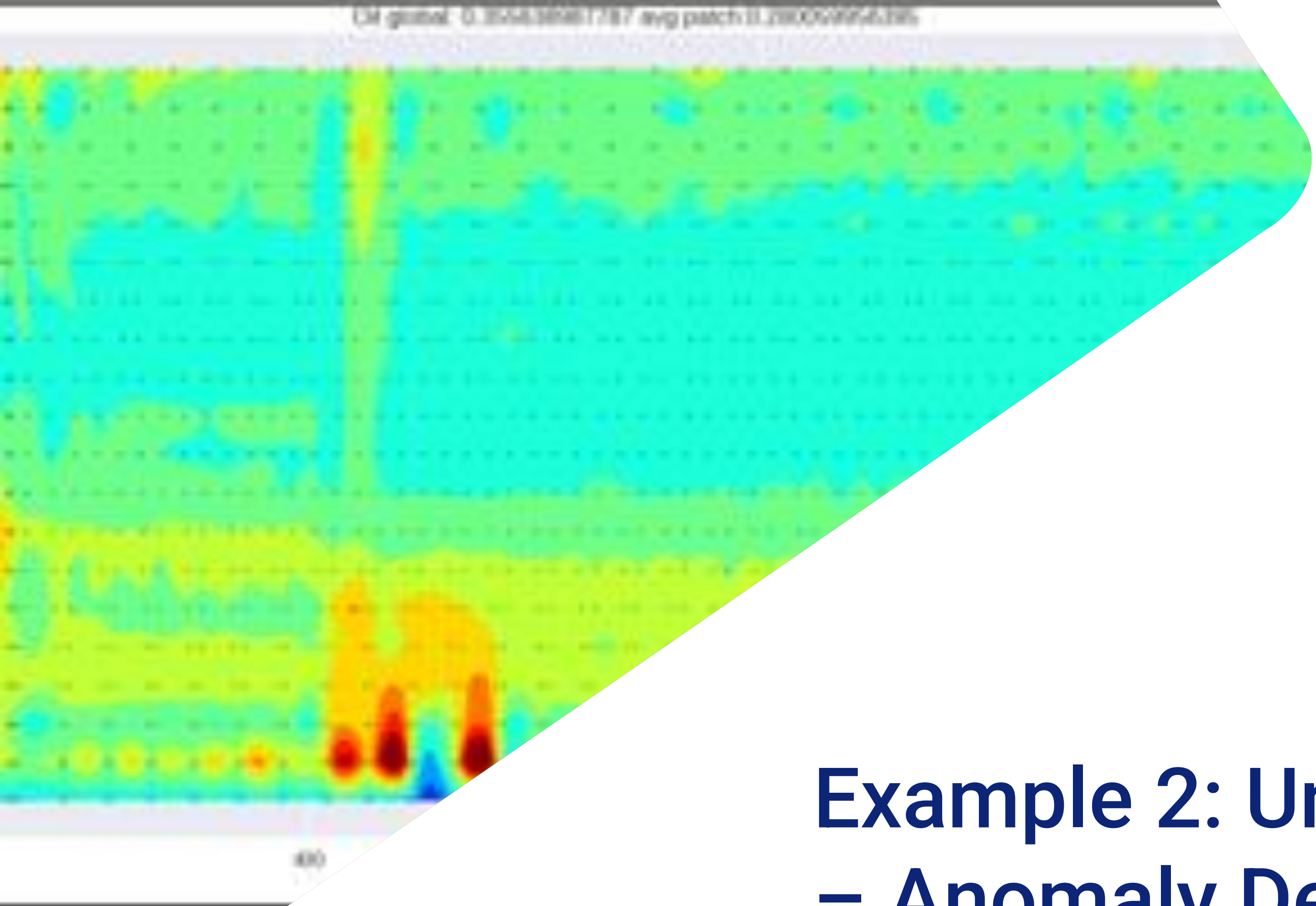

# Results

IOI OLEOCHEMICAL

## Thomas Kummer, IOI Oleo GmbH, Witten, Germany

- “Thanks to the AI-experts, we are now going the crucial step for the optimization of our product. We are very impressed by the results. The cooperation was very pleasant and we experienced the team as highly competent and efficient. We are using this approach also for other products of IOI Oleochemicals and are looking forward to further cooperation. We recommend divis as a competent partner. Next to the professional competence of Thomas Bäck’s team, we are also impressed by their ability to focus on our technical requirements and to employ AI-methods specifically, just as required by the task.”
- More specifically:
  - OOS batches have been reduced from about 50% to 0% → all batches can be sold.
  - IOI decides to roll out data driven analytics to other processes, too.

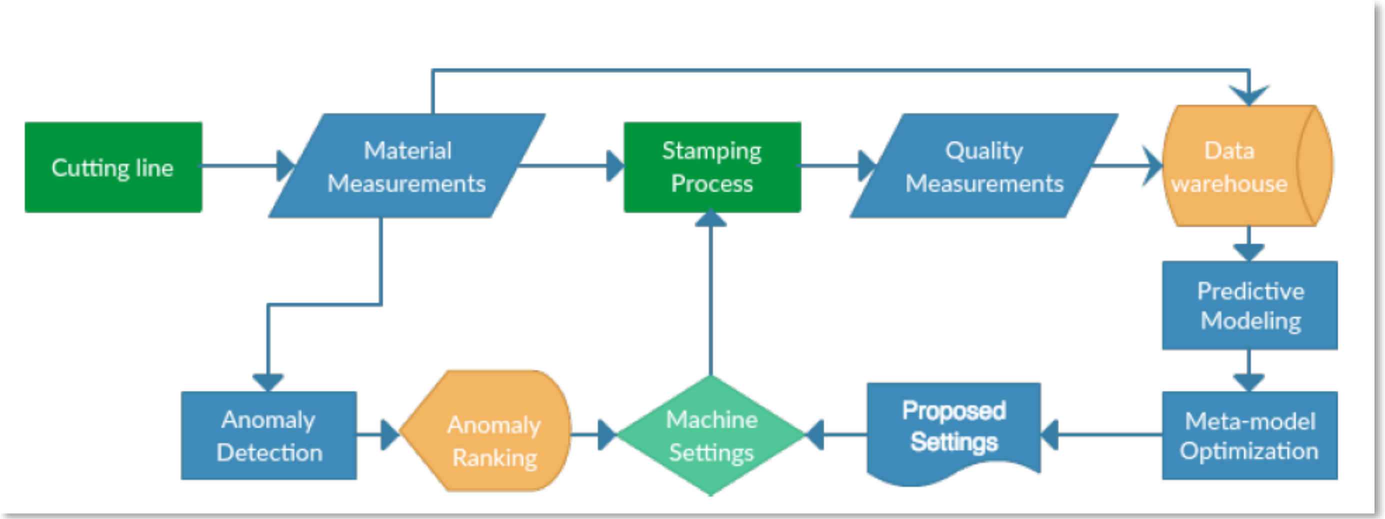
- More information:
  - Process Optimization at IOI Oleo GmbH - divis intelligent solutions GmbH (divis-gmbh.de)
  - Video (in German): Maschinelles Lernen für die Prozessoptimierung: Praxisbeispiel IOI Oleo GmbH - YouTube

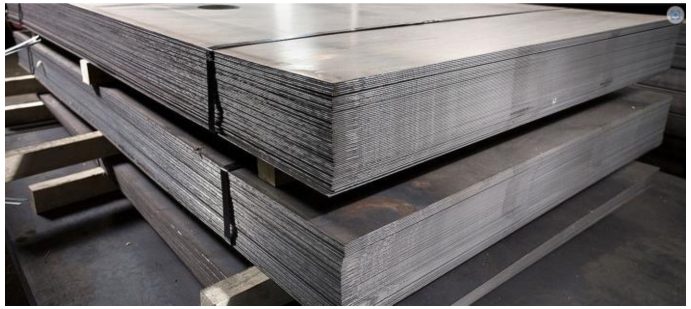


# Example 2: Unsupervised Learning – Anomaly Detection in Coils

# Process Framework

Implementation of data analytics and optimization loop



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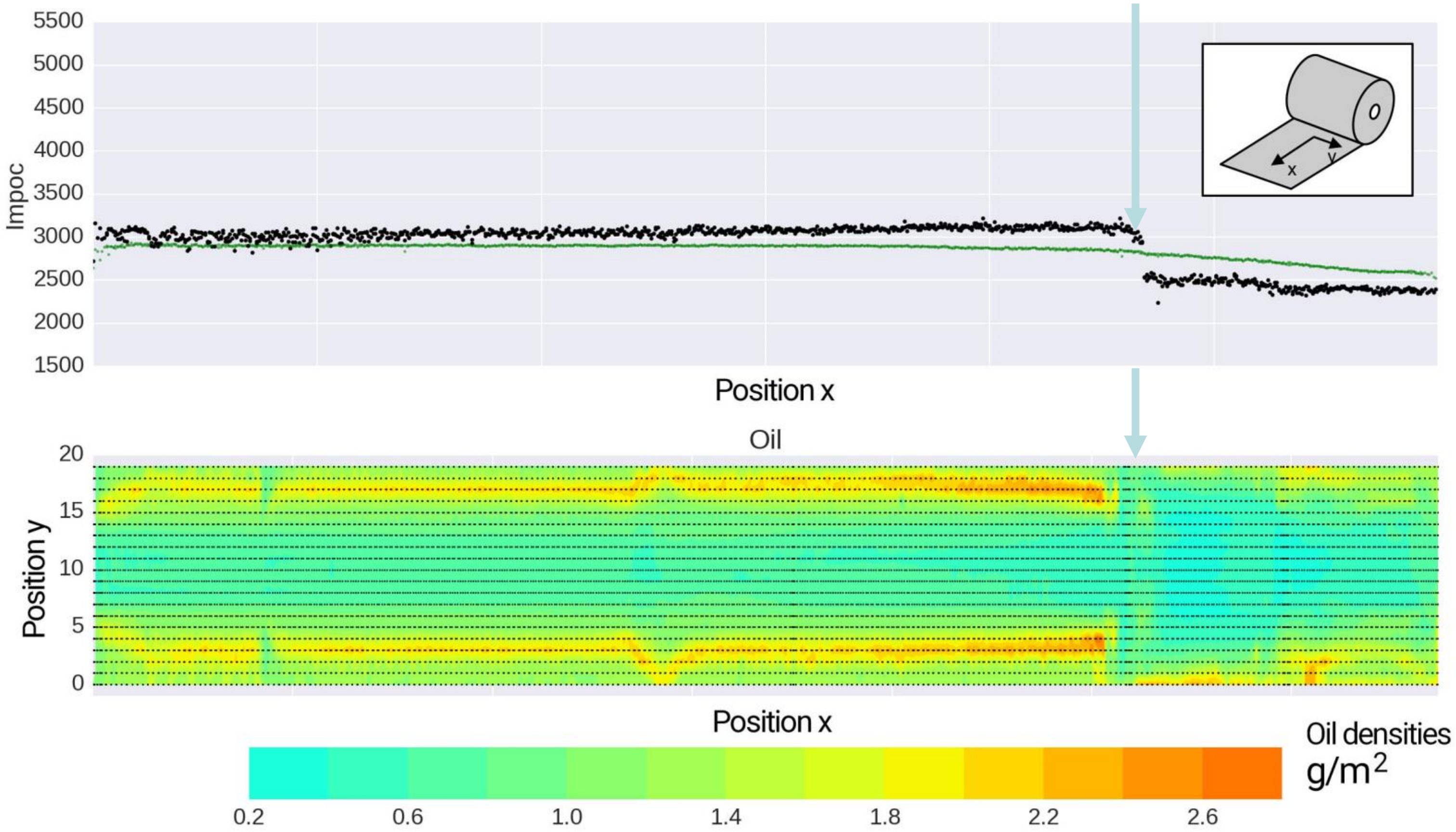
B. van Stein, M. van Leeuwen, H. Wang, S. Purr, S. Kreissl, J. Meinhardt, **Th. Bäck**: Towards Data Driven Process Control in Manufacturing Body Parts. In: *2016 International Symposium on Computational Science and Computational Intelligence, Las Vegas, NV, Dec. 15-17, 2016*, pp. 459-462. IEEE Press, Piscataway, NJ, 2016.

# Exploratory Data Analysis

- Data used:
  - 44 measurement columns
  - Oil
  - IMPOC
  - Thickness
  - Roughness

- This coil:
  - Different production slabs
  - Welded together



# Automated Coil Anomaly Detection

- Idea: Flag „unusual“ coils automatically

**Algorithm 1** GLOSS

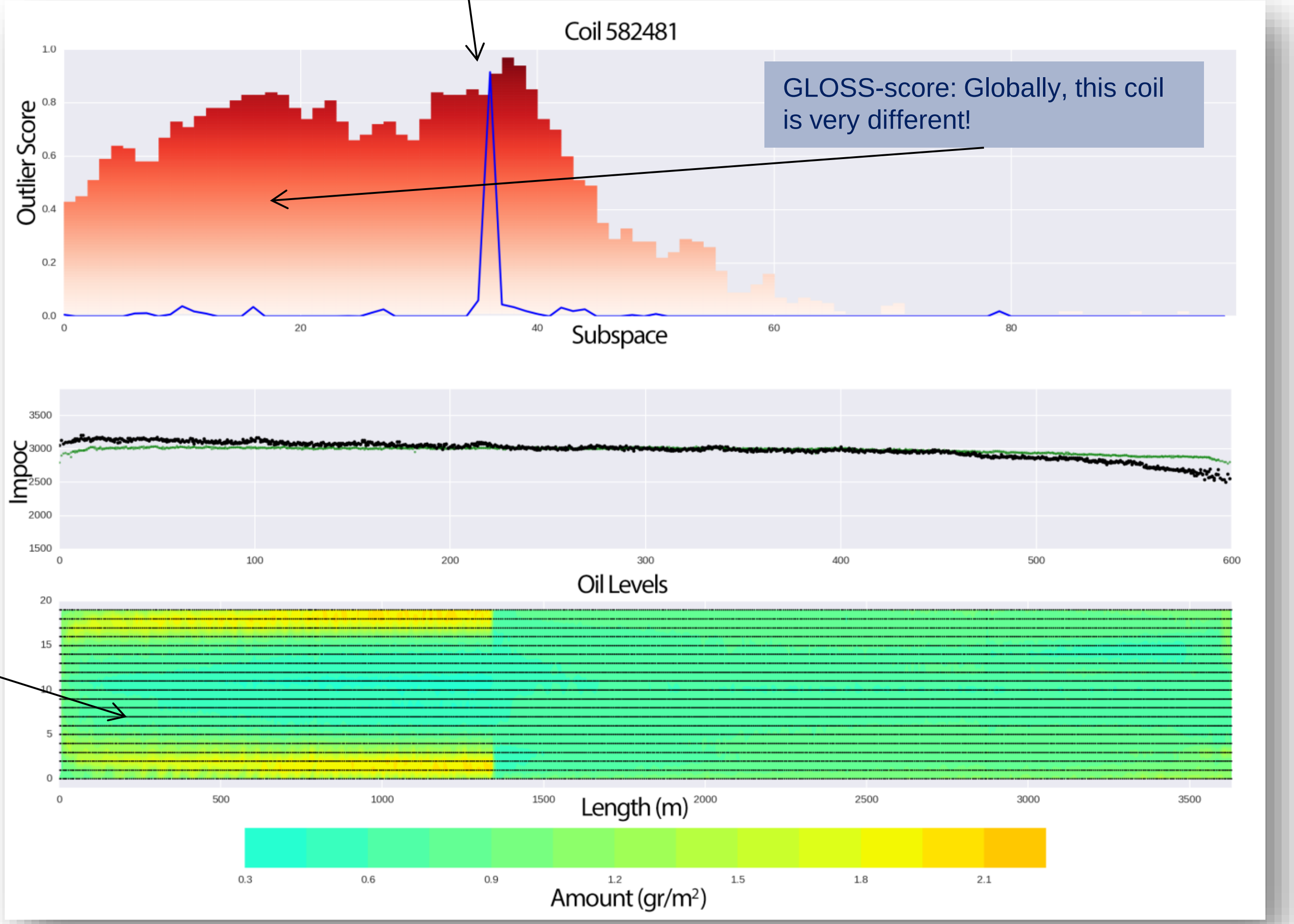
**Given:** Dataset $D$, neighbourhood size $k$, optional: subspaces $\mathcal{F}$

$\mathcal{F} = \text{SubspaceSearch}(D)$ # Only if $\mathcal{F}$ not given
**for all** $d \in D$ **do**:
  $G_d = NN_k(d)$
**for all** $d \in D$ **do**
  **for all** $F \in \mathcal{F}$ **do**
    $\sigma(d_F, G_d) = \sqrt{\frac{\sum_{s \in G_d} \text{dist}(d_F, s_F)^2}{|G_d|}}$
    $\text{pdist}(\lambda, d_F, G_d) = \lambda \cdot \sigma(d_F, G_d)$
    $PGLOF_{\lambda, G_d}(d_F) = \frac{\text{pdist}(\lambda, d_F, G_d)}{\mathrm{E}_{s \in G_d}[\text{pdist}(\lambda, s, G_s)]} - 1$
    $p_{F,k}(d) = \max\left\{0, \text{erf}\left(\frac{PGLOF_{\lambda, G_d}(d_F)}{nPGLOF \cdot \sqrt{2}}\right)\right\}$
**return** $p$

LoOP-score: Detects only a local outlier

GLOSS-score: Globally, this coil is very different!

GLOSS-score: Globally, high oil levels at the beginning are very unlikely!




B. van Stein, M. van Leeuwen, H. Wang, S. Purr, S. Kreissl, J. Meinhardt, T. Bäck: **Towards data driven process control in manufacturing car body parts**. IEEE CSCI Conference, 459-462, 2016.

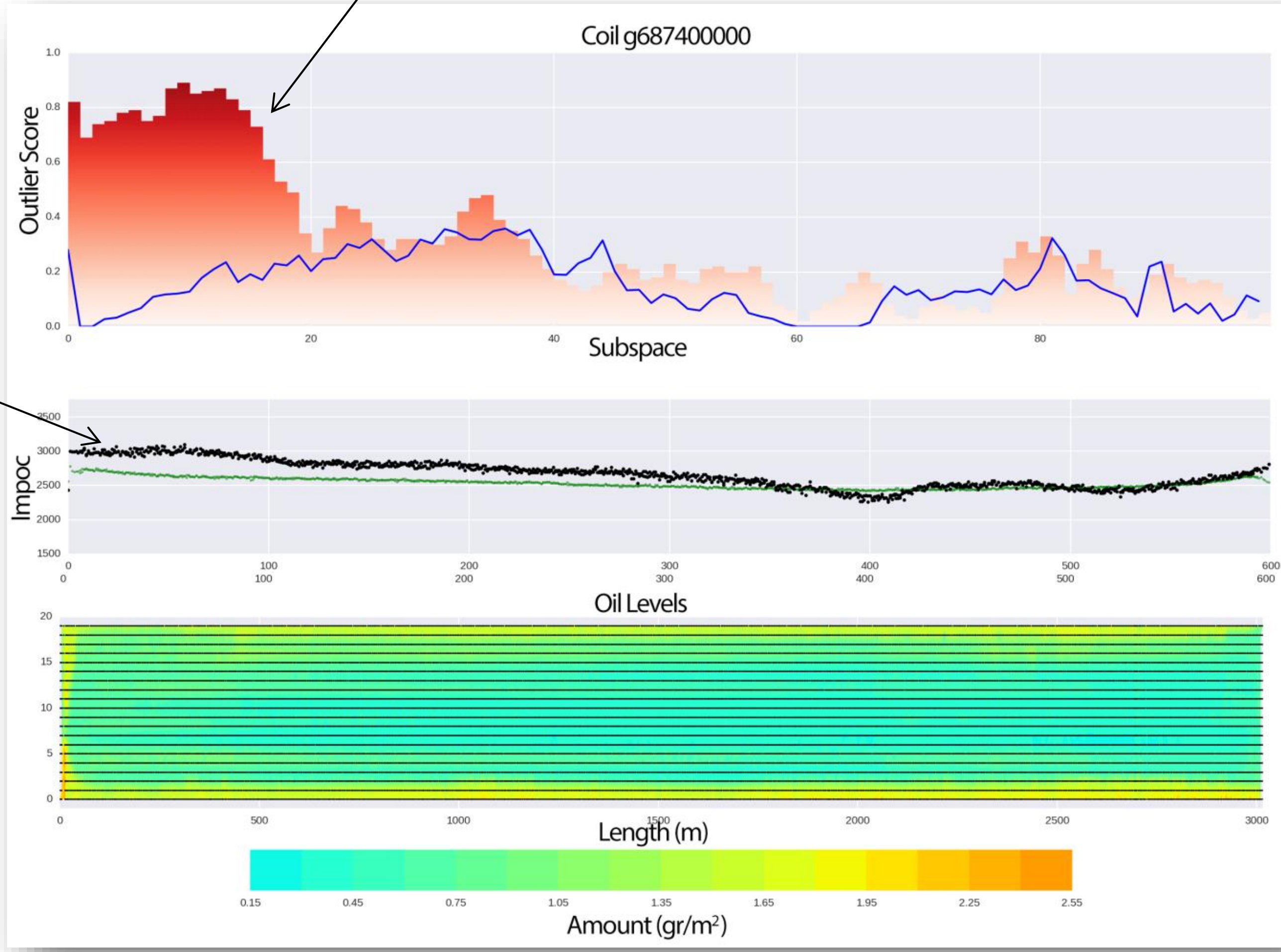
# Automated Coil Anomaly Detection: 3rd Example

- A less obvious anomaly
- Correctly detected

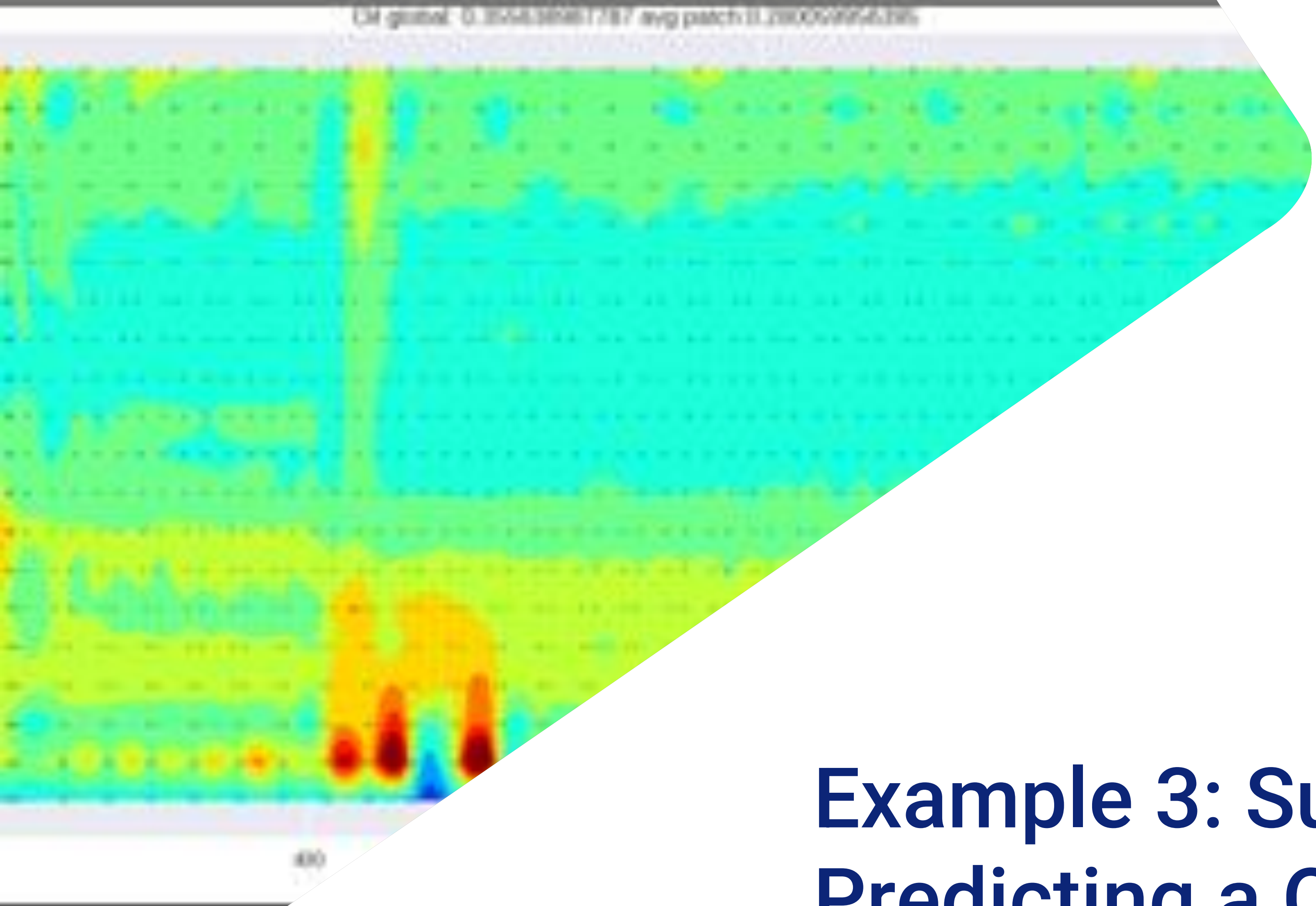
- Research project 2014 - 2019

GLOSS-score: Globally, this coil is very different!

GLOSS-score: Impoc deviates a lot from global neighbors!



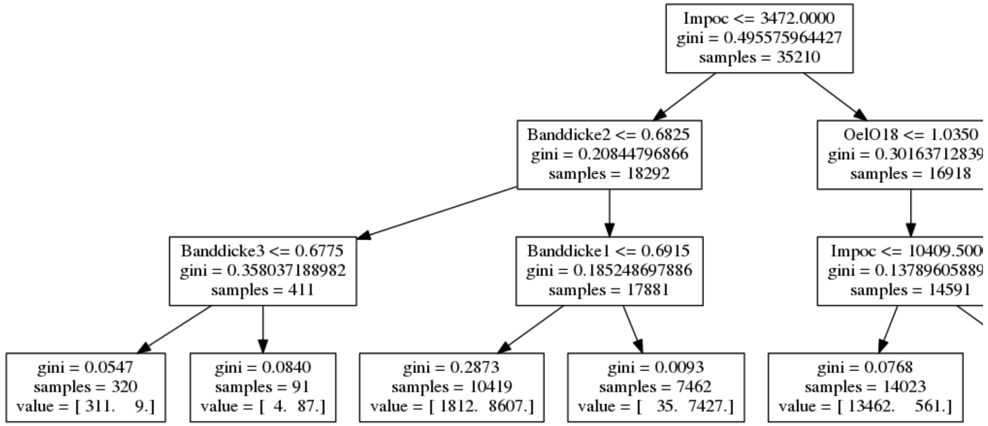

B. van Stein, M. van Leeuwen, H. Wang, S. Purr, S. Kreissl, J. Meinhardt, T. Bäck: **Towards data driven process control in manufacturing car body parts**. IEEE CSCI Conference, 459-462, 2016.

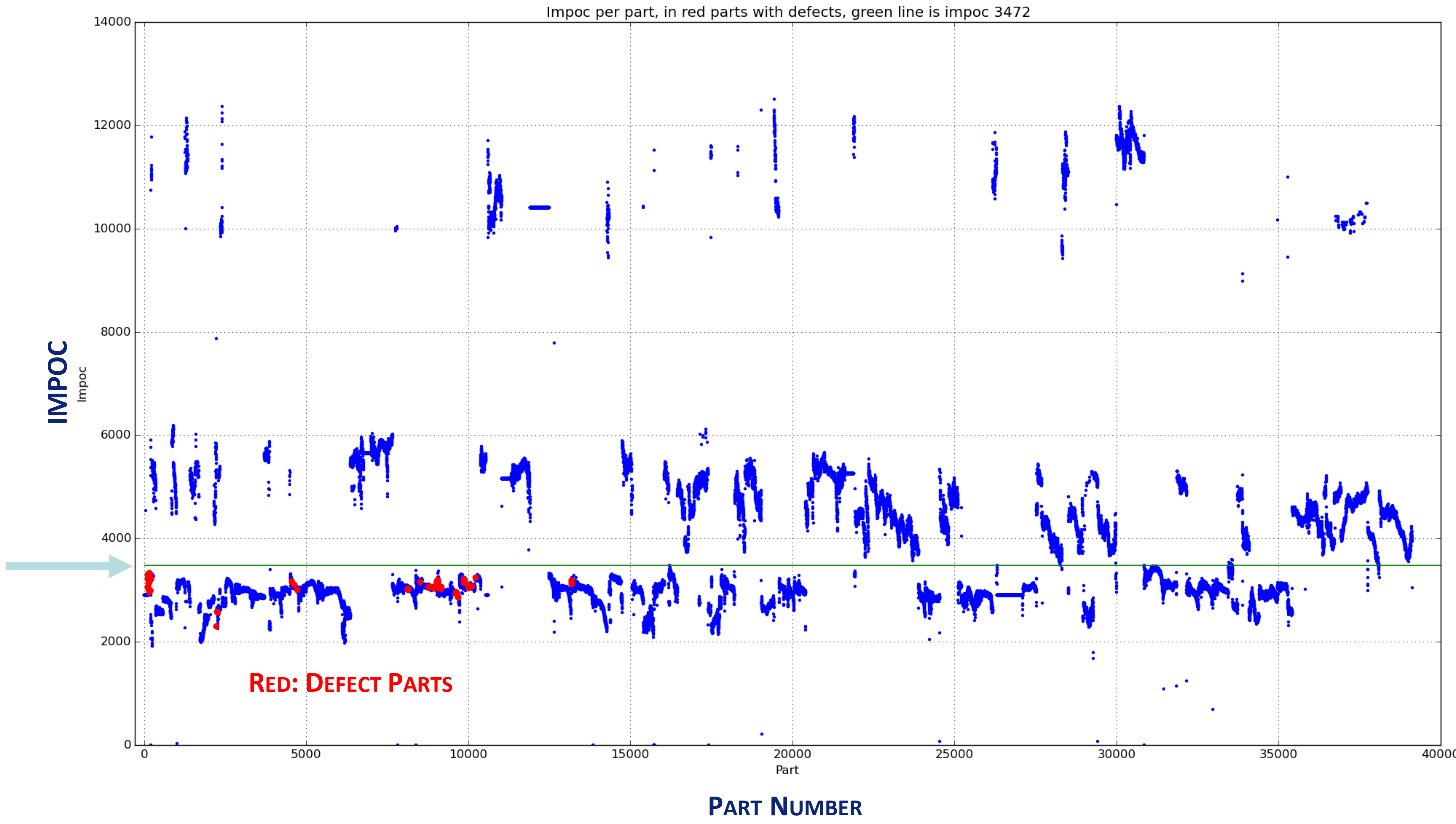


# Example 3: Supervised Learning – Predicting a Quality Measure

# Machine Learning: Decision Tree

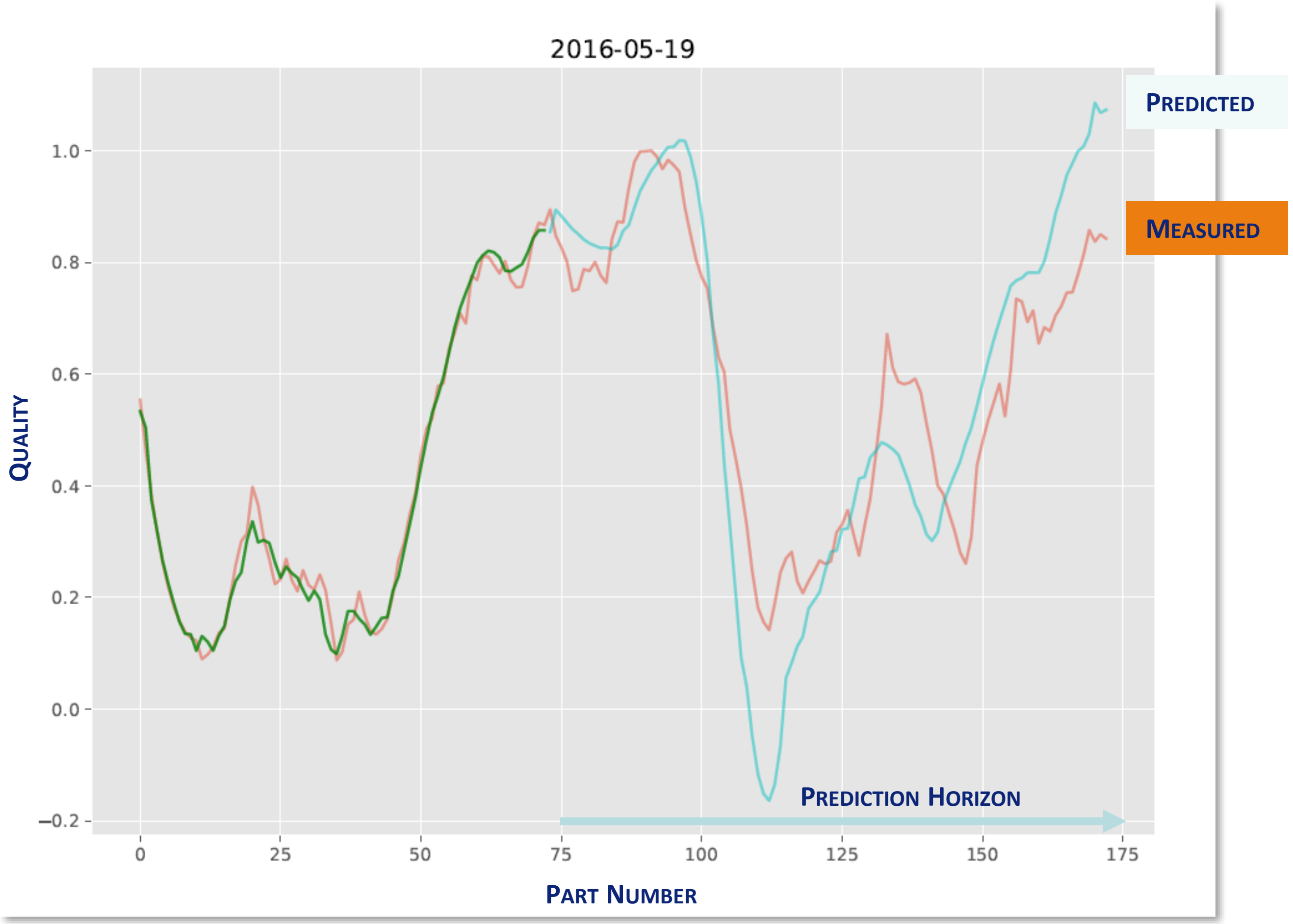
- Quality measure: Class (OK/NOK)
- Most important split:
  - IMPOC value

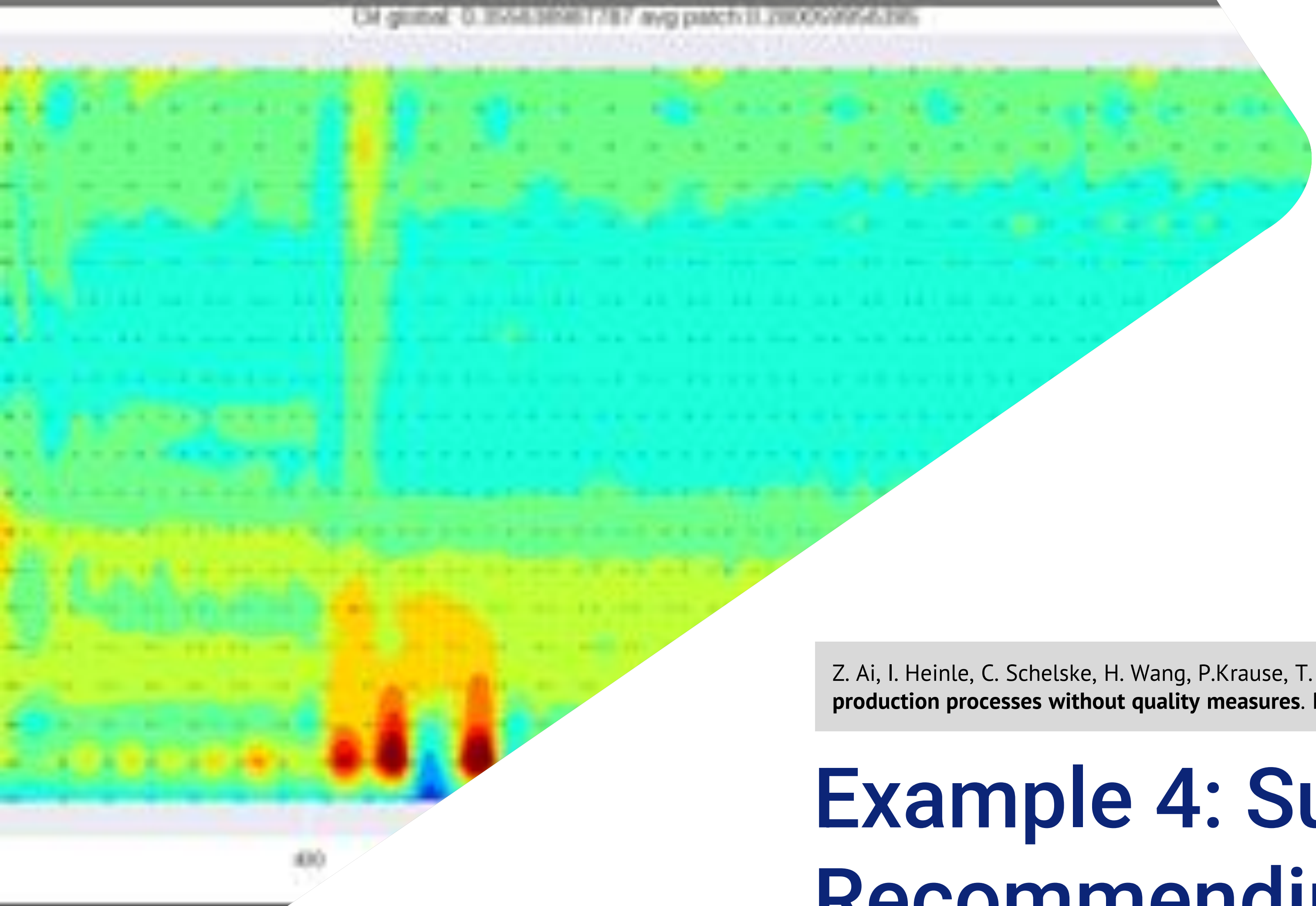


# Training a Model – Validation – Prediction

- Data used: as before
- Precision measure
  - Indent …
  - Continuous measure
- Prediction for 100 parts into future
  - Knowing the stack order
  - Therefore knowing the material parameters
  - Fixed cylinder forces



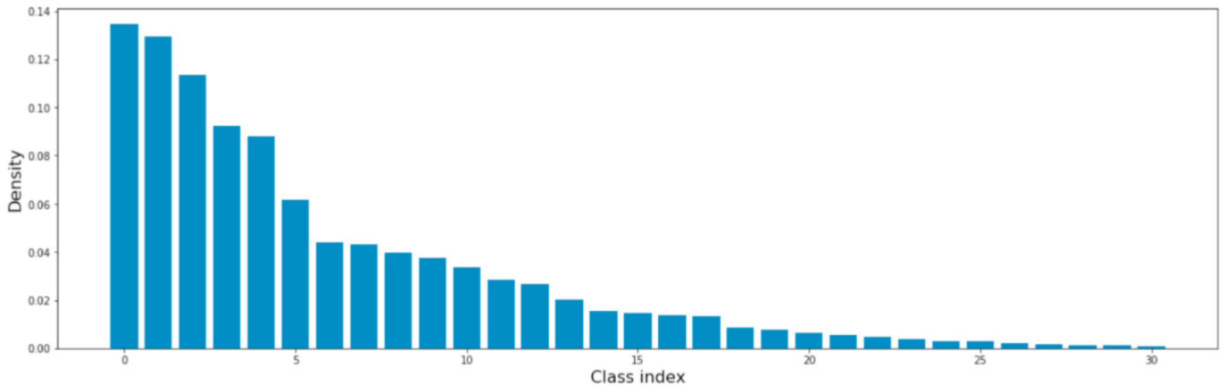



Z. Ai, I. Heinle, C. Schelske, H. Wang, P.Krause, T. Bäck: **A classification-based solution for recommending process parameters of production processes without quality measures**. Procedia Computer Science 180, 600-607, 2021

# Example 4: Supervised Learning for Recommending Process Parameters

# Current Situation

- Stamping process of parts: Difficult to find good process parameters
- Parameter changes are carefully made → only few variations available




- Lack of inline quality data → difficult to learn relation between blank properties, process parameters and quality

# Idea: Recommending Process Parameters

- Select best fitting known process parameter combination for a given blank / stack

Determine successful combinations of blank properties & process parameters

**Process control based on part quality**

Parts fulfilling quality standards → Successful combination parameters & blank properties

Geometrical deviation
- Below threshold
- …

**Process control without part quality**

"Normal" blank properties + Stationary production conditions → Successful combination parameters & blank properties

Anomaly detection
- Oil
- Thickness
- Roughness
- IMPOC
- …

Rules
- Ignore first blank
- …

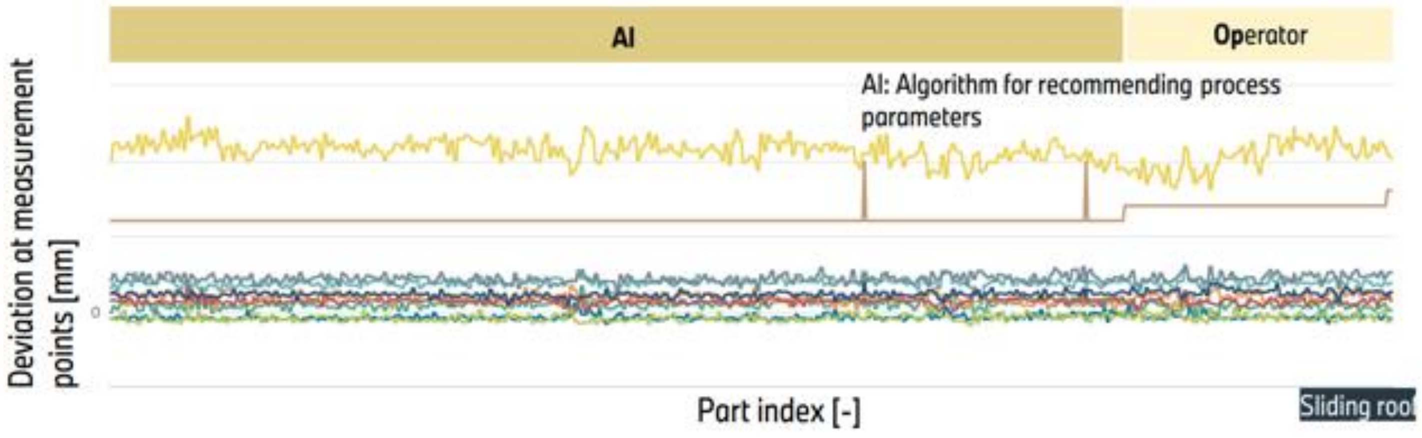
- Training: Blank + Process → Quality = good
- Deploy: Blank → Process

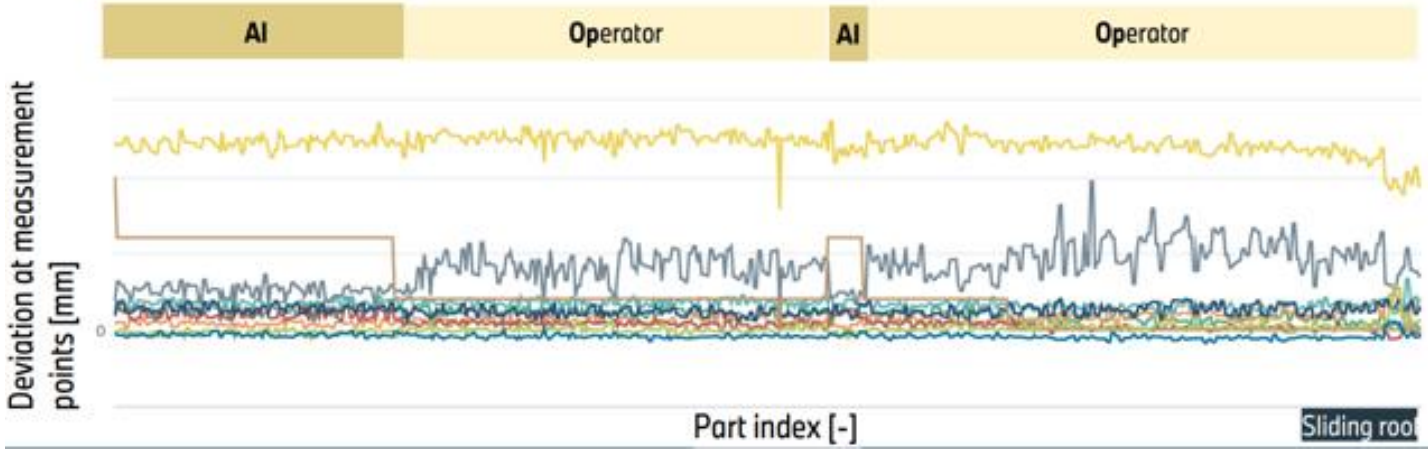
| | Algorithm based on PART QUALITY | Algorithm WITHOUT PART QUALITY |
|---|---|---|
| Accuracy* | 93.06% | 92.47% |
| Weighted F1 Score** | 92.52% | 91.83% |

* Accuracy = (TP + TN) / (TP + TN + FP + FN) True Positives, True Negatives, False Positives, False Negatives

** F1 = 2 x Precision x Recall / (Precision + Recall) Precision = TP / (TP + FP); Recall = TP / (TP + FN)

# Deployed Application



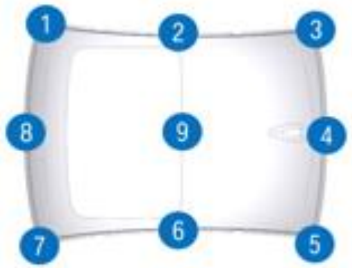




Chosen cushion cylinder forces

| Cyl. [-] | Op. [kN] | AI [kN] |
|---|---|---|
| 1 | 160 | 160 |
| 2 | 270 | 260 |
| 3 | 160 | 160 |
| 4 | 270 | 260 |
| 5 | 180 | 160 |
| 6 | 270 | 260 |
| 7 | 180 | 160 |
| 8 | 270 | 260 |

| Cyl. [-] | Op. [kN] | AI [kN] |
|---|---|---|
| 1 | 160 | 160 |
| 2 | 220 | 260 |
| 3 | 160 | 160 |
| 4 | 220 | 260 |
| 5 | 160 | 160 |
| 6 | 220 | 260 |
| 7 | 160 | 160 |
| 8 | 220 | 260 |

**Measurement points geometry**




**Legend deviation between target geometry and measured value**

— 1 — 2 — 3
— 4 — 5 — 6
— 7 — 8 — 9

**Process parameters**

Only the 8 cushion cylinder forces are changed during production

— Scaled change force cylinder 2

# EVOLUTIONARY OPTIMIZATION IN PRODUCT DEVELOPMENT

# Discovery in Vitro

- MacMillan – Rabitz groups, about 2008
- Dr. Ofer Shir, LIACS
- Algorithmically guided organic synthesis: Reaction optimization

Goal: optimize the reaction of a pharmaceutical building block


- Decision variables (7 categorical variables):
  *3 projected indoles, 5 photo-catalysts, 5 discrete molarities, 16 solvents, 5 discrete stoichiometries, 16 bases, 12 additives*
- Search-space cardinality: ~$10^6$ combinations
- Robotic setup:
  - *96-well plates for performing screening in parallel*
  - *reaction evaluation per plate within ~48 hours*
- Overall budget of ~1000 reactions (10 iterations)

Approach: a *categorical heuristic search* in a feedback loop

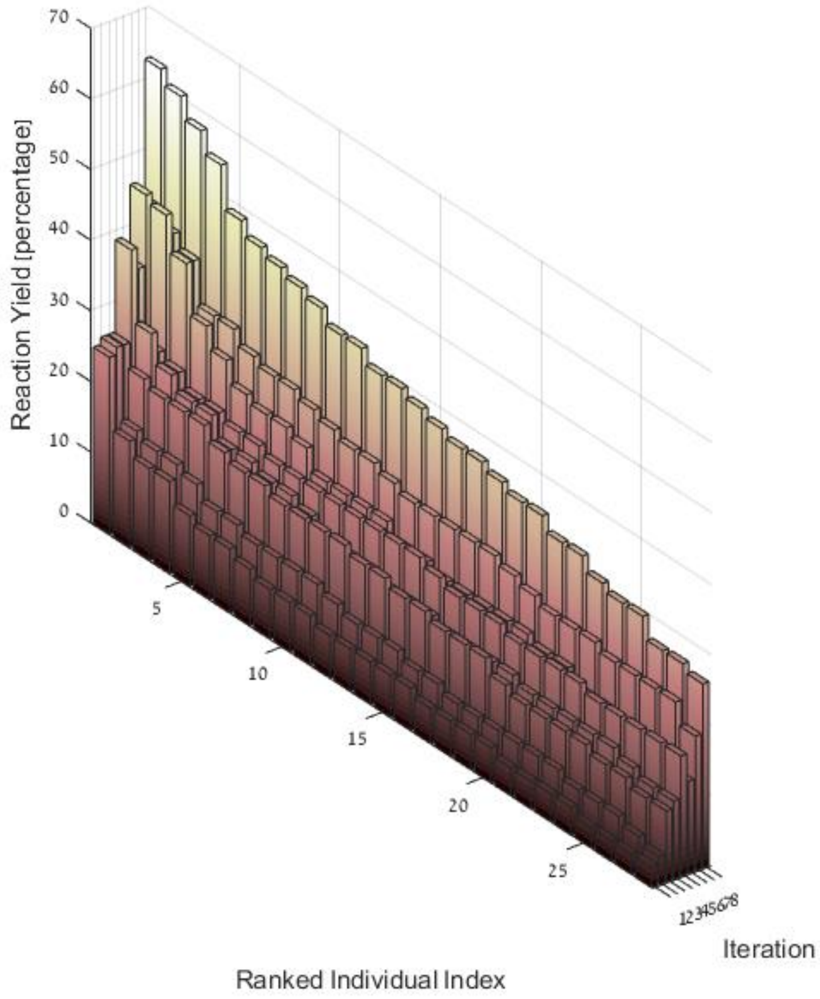
# Organic Synthesis: Results

- We designed an **evolutionary algorithm** to address this experimental combinatorial optimization problem.

- Depicted: The upper $30^{th}$ percentile of the 96-well plate over 8 iterations.

- The quality of the reaction yield (~65%) was significantly better than the expert's best known reaction (~15%)

- The resultant reaction was of surprising nature, yet, this may not be considered serendipity!



# Mixed-Integer Evolution Strategies

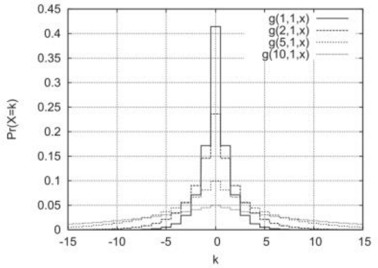



Figure 1: 2D representation of the distribution obtained as the difference of two geometrical distributions for different values of $\varphi$.

Continuous parameters:

**for** $i = 1, \ldots, n_r$ **do**
  $s_i' \leftarrow s_i \exp(\tau_g \mathrm{N}_g + \tau_l \mathrm{N}(0,1))$
  $r_i' = r_i + N(0, s_i')$
**end for**

Discrete parameters:

**for** $i = 1, \ldots, n_z$ **do**
  $q_i' \leftarrow q_i \exp(\tau_g \mathrm{N}_g + \tau_l \mathrm{N}(0,1))$
  $z_i' \leftarrow z_i + \mathrm{G}(0, q_i')$
**end for**

Categorical parameters:

$p_i' := 1/[1 + \frac{1-p_i}{p_i} * \exp(-\tau_l * \mathrm{N}(0,1))]$
**for** $i \in \{1, \ldots, n_d\}$ **do**
  **if** $\mathrm{U}(0,1) < p_i'$ **then**
    $d_i' \leftarrow$ uniformly randomly value from $D_i$
  **end if**
**end for**

Learning rates (global)

Learning rates (local)

Geometrical distribution

Mutation probabilities

- Simple message: Can be used as experimental optimizer

# CONCLUDING

# Conclusions

- AI-based quality control and process optimization have huge potential
- Applicable for batch- and continuous production processes
- Combination of modeling, prediction, and optimization

- Questions?

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