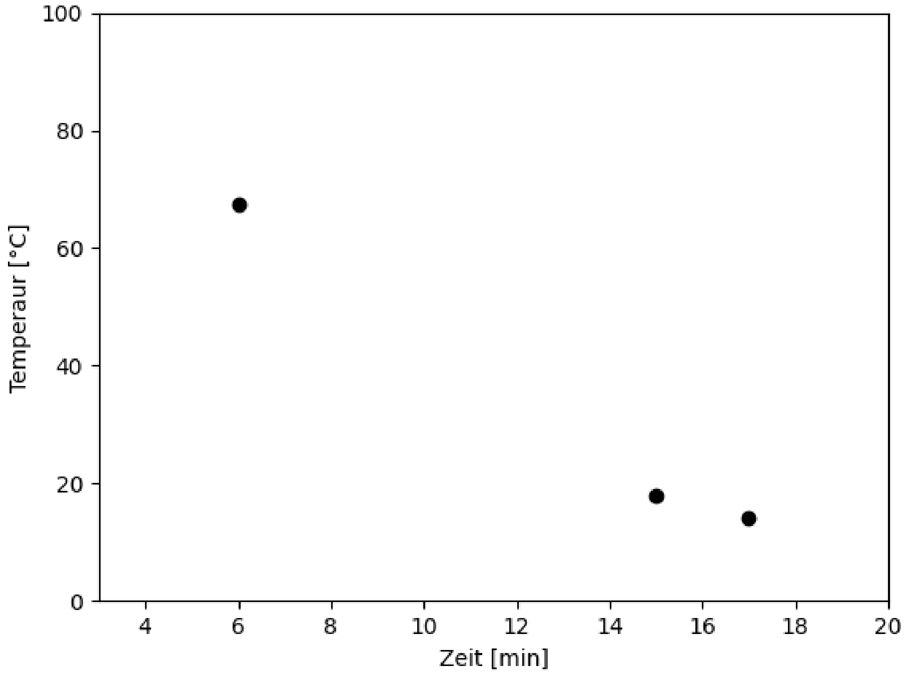
Miltiadis Poursanidis

Shape-Constrained Regression

Introductory Example

Regression in a Few Data Setting



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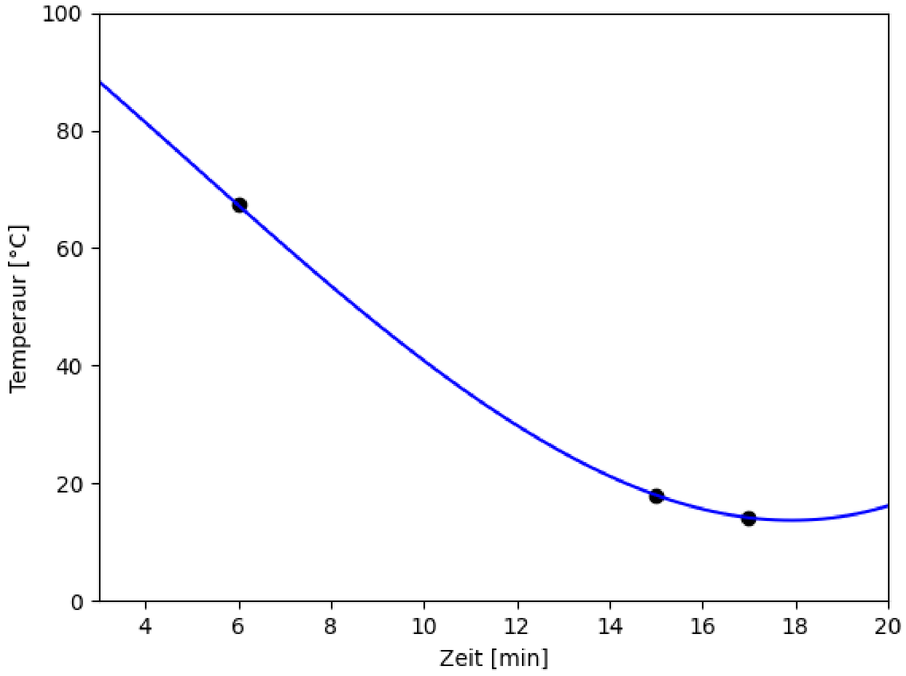

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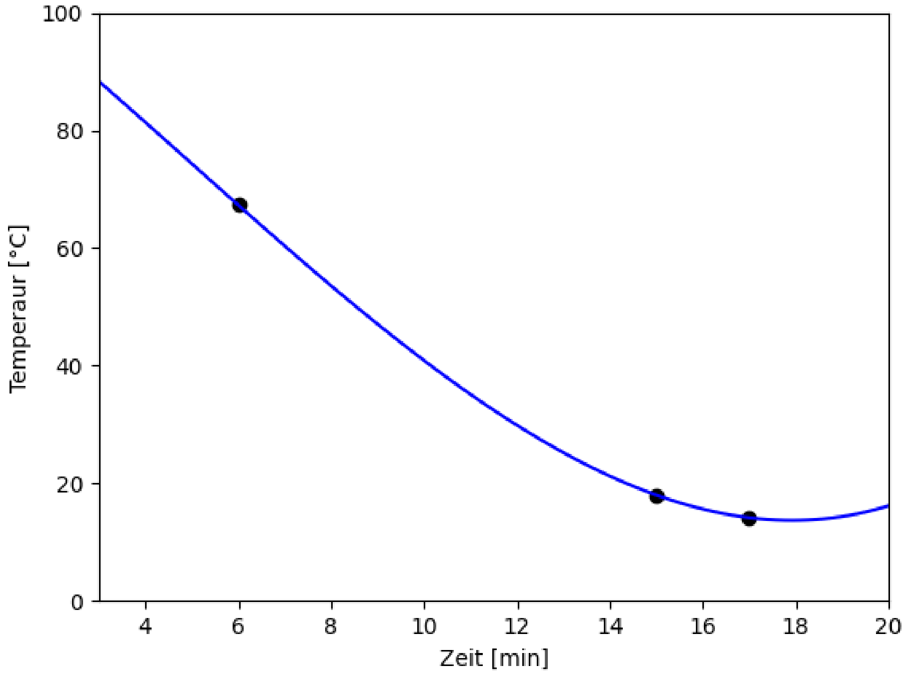

Challenges:

- Noisy data (measurement errors, uncollected variables)
- Few data (cost money and time)

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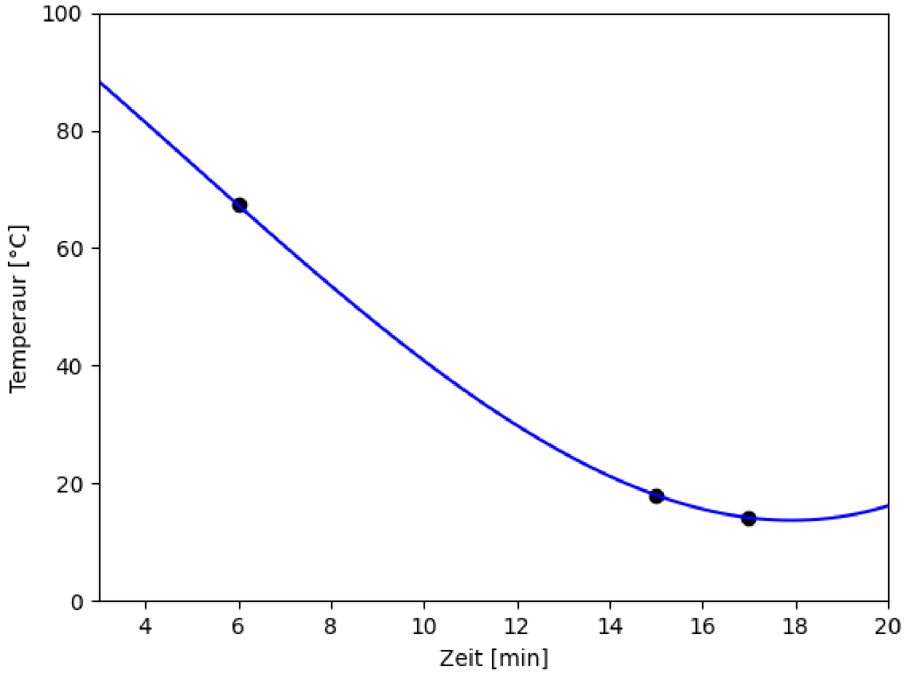

Data-based Modeling

- Often unphysical
- Often not trustworthy

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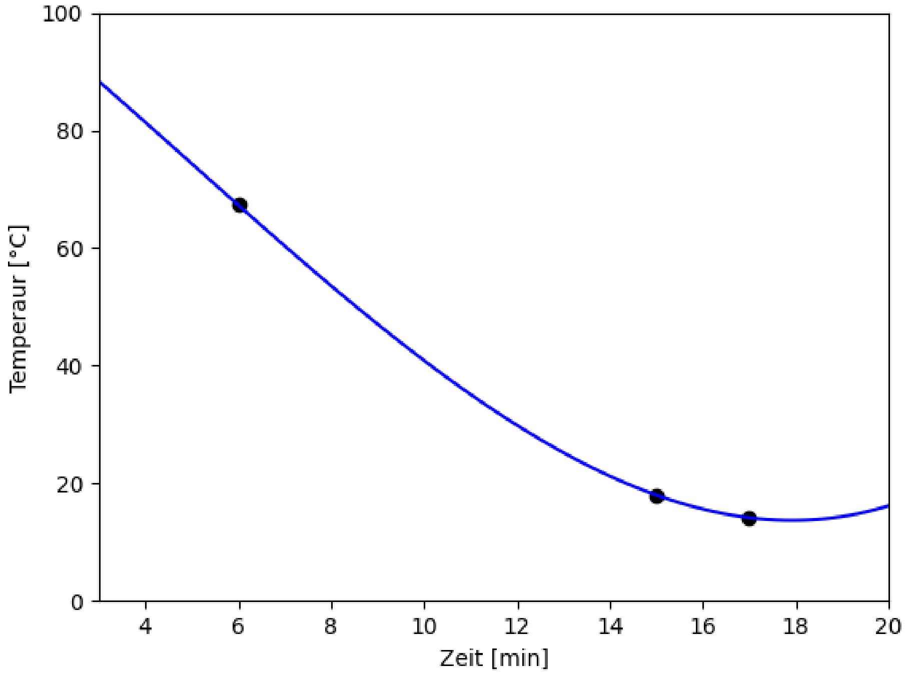

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Integration of Prior Knowledge (here Decreasingness):

- Physically consistent
- Less data required
- Compensating noise of data

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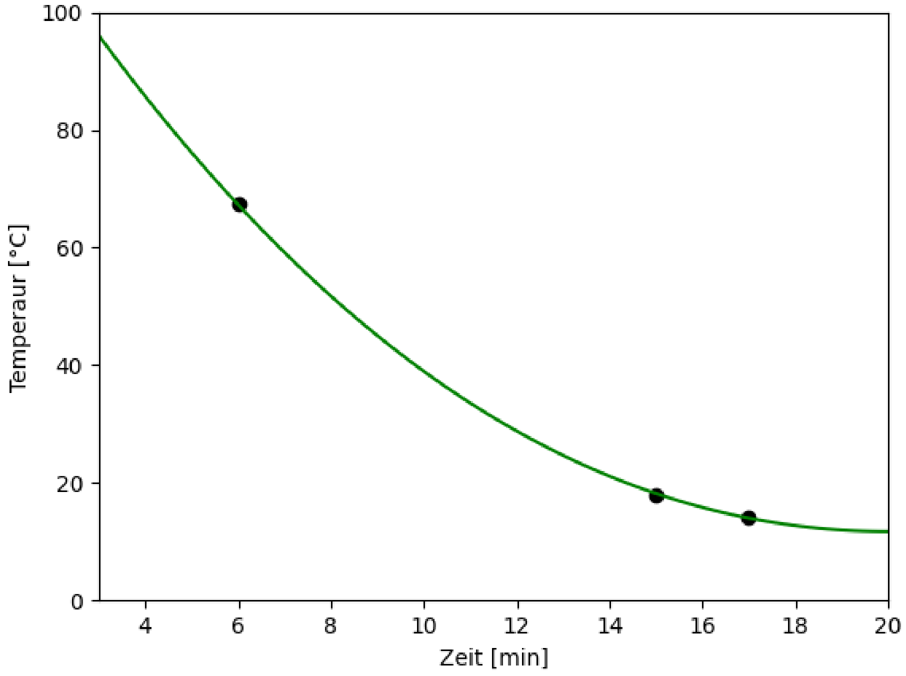

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Theory

Problem Statement
Shape-Constrained Regression

Consider:

$$\min_{w \in W} \sum_{l=1}^{N} \left(y^l - \hat{y}(w, x^l)\right)^2 + \lambda |w|^2$$

 24.01.2025

Problem Statement

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$$s.t. \;\; \partial_{x_j} \hat{y}(w, x) \leq 0, \qquad (x \in X)$$

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$$\min_{w \in W} \sum_{l=1}^{N} \left(y^l - \hat{y}\left(w, x^l\right)\right)^2 + \lambda |w|^2$$

$$s.t.\ \ \psi_i\left((\partial_x^\alpha \hat{y}(w,x))_{|\alpha|_1 \leq 2}\right) \leq 0, \qquad (x \in X, i \in I),$$

Problem Statement

Shape-Constrained Regression

Consider:

$$\min_{w\in W} \overbrace{\sum_{l=1}^{N}\left(y^l - \hat{y}(w,x^l)\right)^2 + \lambda|w|^2}^{= f(w)}$$

$$s.t.\ \underbrace{\psi_i\left((\partial_x^\alpha \hat{y}(w,x))_{|\alpha|_1\leq 2}\right)}_{= g_i(w,x)} \leq 0, \qquad (x \in X, i \in I),$$

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As a *Semi-Infinites Optimization Problem:*

$$\text{SIP:} \qquad \min_{w \in W} f(w) \qquad s.t.\ \ g_i(w,x) \leq 0, \qquad (x \in X, i \in I).$$

Algorithm to Solve SIPs
Core Algorithm

Input: $\boldsymbol{\varepsilon} \geq 0$ *(restriction parameter)*, $\boldsymbol{\rho} \in [0, \infty]$ *(exchange parameter)*, $\boldsymbol{X^0} \subset X$ finite *(initial discretization)*, $\overline{\delta}, \underline{\boldsymbol{\delta}} \geq 0$ *(approximation error of upper and lower level)*

1. Set $k = 0$ and $X^k = \boldsymbol{X^0}$
2. Find a $\overline{\delta}$-optimal solution w^k of the *upper-level problem:*
   $$OSP(X^k): \quad \min_{w \in W} f(w) \quad s.t. \quad g(w, x) \leq -\boldsymbol{\varepsilon}, \ \forall x \in X^k.$$
3. Find a $\underline{\boldsymbol{\delta}}$-optimal solution x^k of the *lower-level problem:*
   $$USP(w^k): \quad \max_{x \in X} g(w^k, x)$$
4. If $g(w^k, x^k) \leq -\underline{\boldsymbol{\delta}}$:
   - Terminate and return w^k
5. Else:
   - Set $X^{k+1} := \{x \in X^k : g(w^k, x) \geq -\boldsymbol{\varepsilon} - \boldsymbol{\rho}\} \cup \{x^k\}$
   - Set $k := k + 1$ and jump to step 2

Python-Package

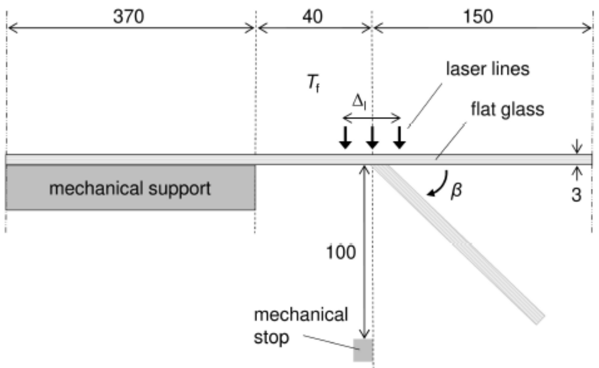
SIASCOR

```python
shape_constraints = [
    LowerBoundConstraint(0),
    UpperBoundConstraint(1),
    MonotonicityConstraint(0),
    MonotonicityConstraint(3, decreasing=True),
    ConvexityConstraint(2),
]
siascor_model = Siascor(
    features=PolynomialFeatures(degree=4), shape_constraints=shape_constraints
)
siascor_model.fit(X, y)
```

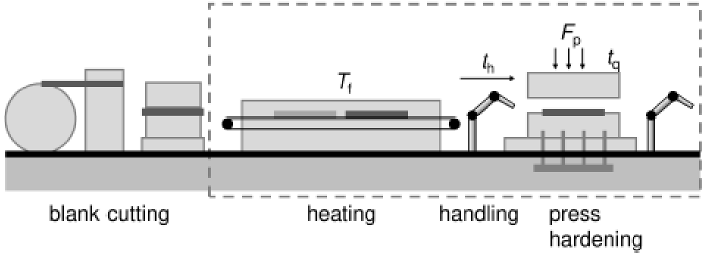
Applications

Applications

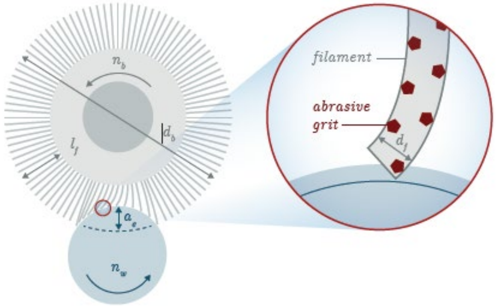
From Manufacturing



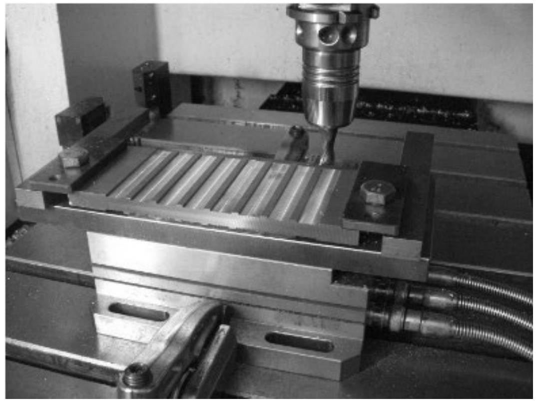
Glas Bending



Press Hardening



Brushing



Milling

- Goal: Find a function that models product quality w.r.t. process parameters

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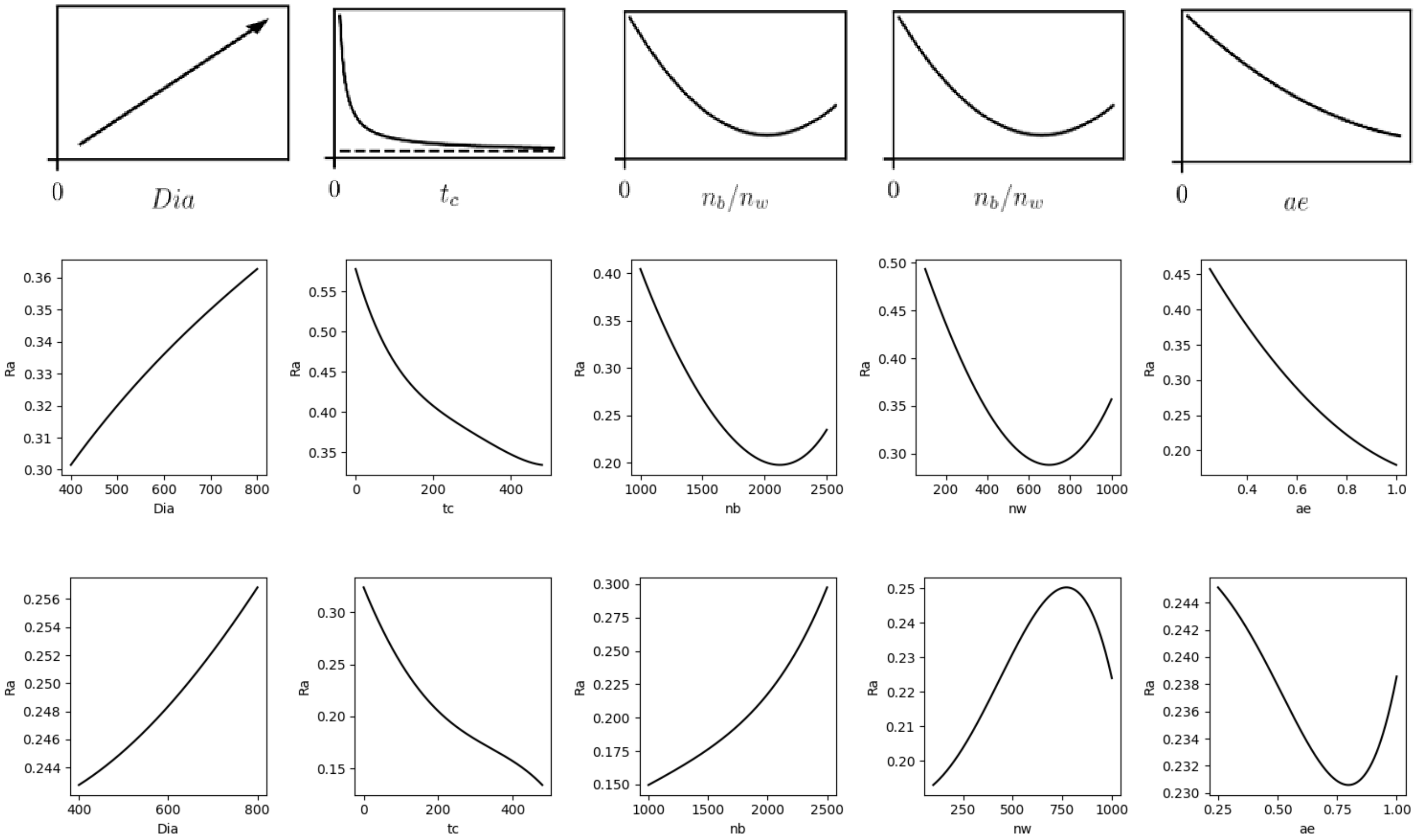
Results

Shape-constrained Regression for the Brushing Example

Shape-Constraints

Shape-Constrained Model

Unconstrained Model



Thank you!

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