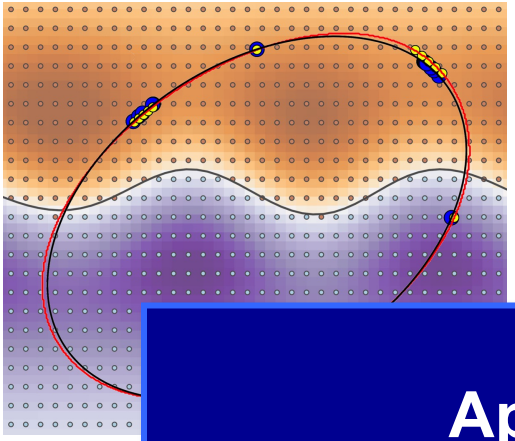

14.11.2022

Applications of Machine Learning to Mechanical Systems

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RUHR UNIVERSITÄT BOCHUM

RUB

Outline

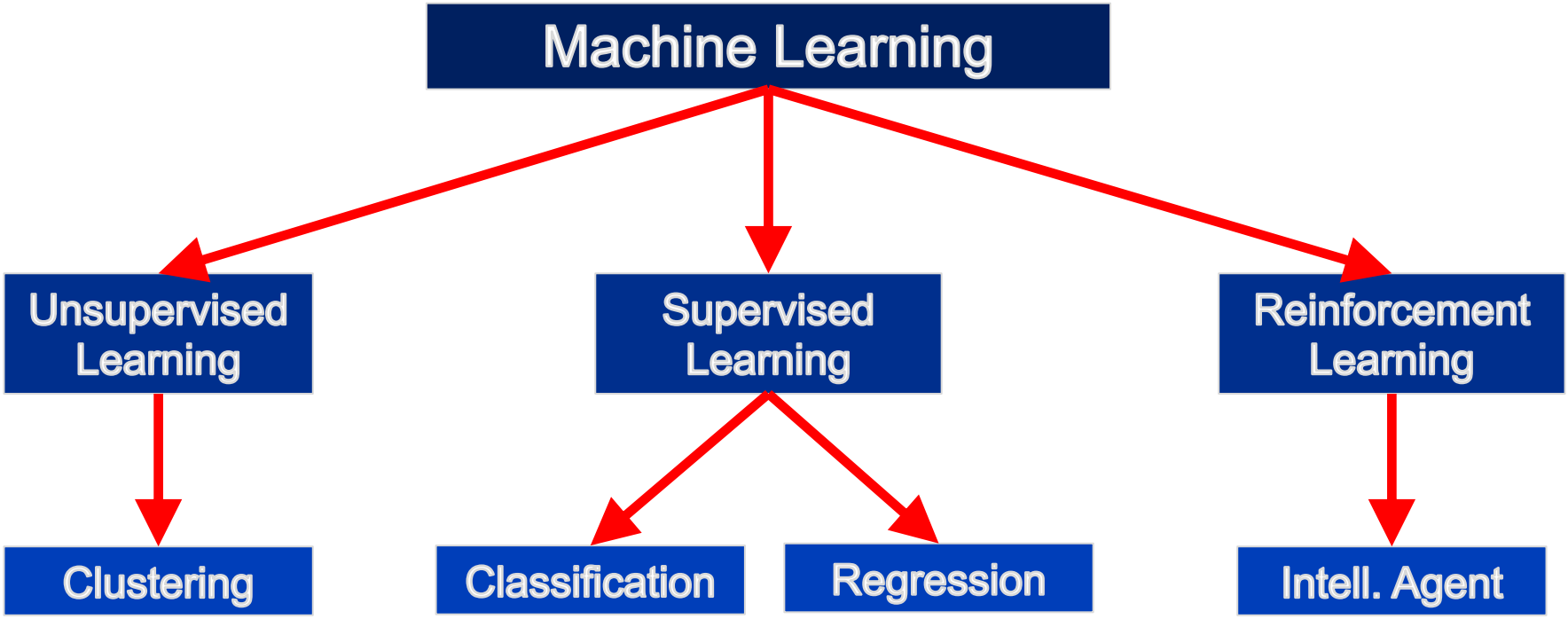
I. Lecture
   1. Machine Learning (ML) methods
   2. Applications as surrogate models for indentation
   3. Learning microstructure-property relationships

II. Tutorials
   1. ML-Classification
   2. ML-Regression

   Use tutorials on MyBinder.org launch binder

   Installation from GitLab repository:
   https://gitlab.ruhr-uni-bochum.de/hartmajg/ml-tutorial.git

Machine Learning (ML)



All examples of this lecture have been performed with scikit-learn (https://scikit-learn.org/stable/)

Reinforcement Learning: Intelligent Agents

Task: Create a computer code that can play “Go”

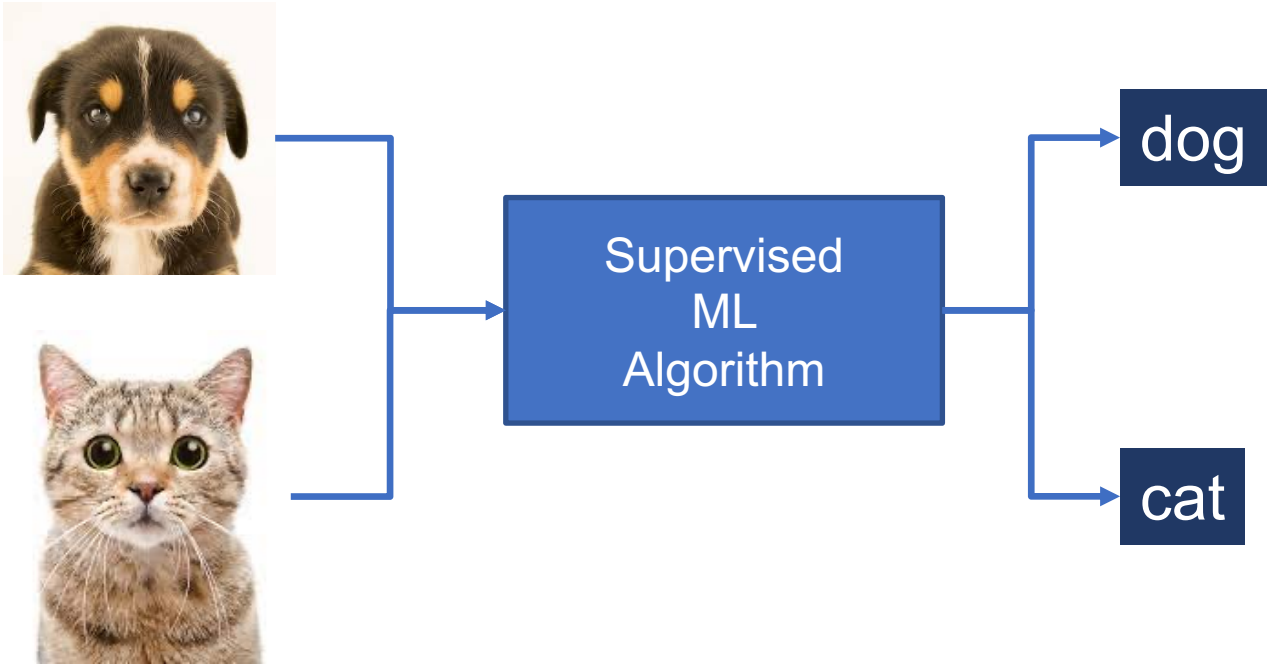
Source: Wikipedia
Wikimedia Commons, CC BY-SA 3.0

Unsupervised Learning: Clustering

Task: Sort pictures of same animals into groups (clustering)

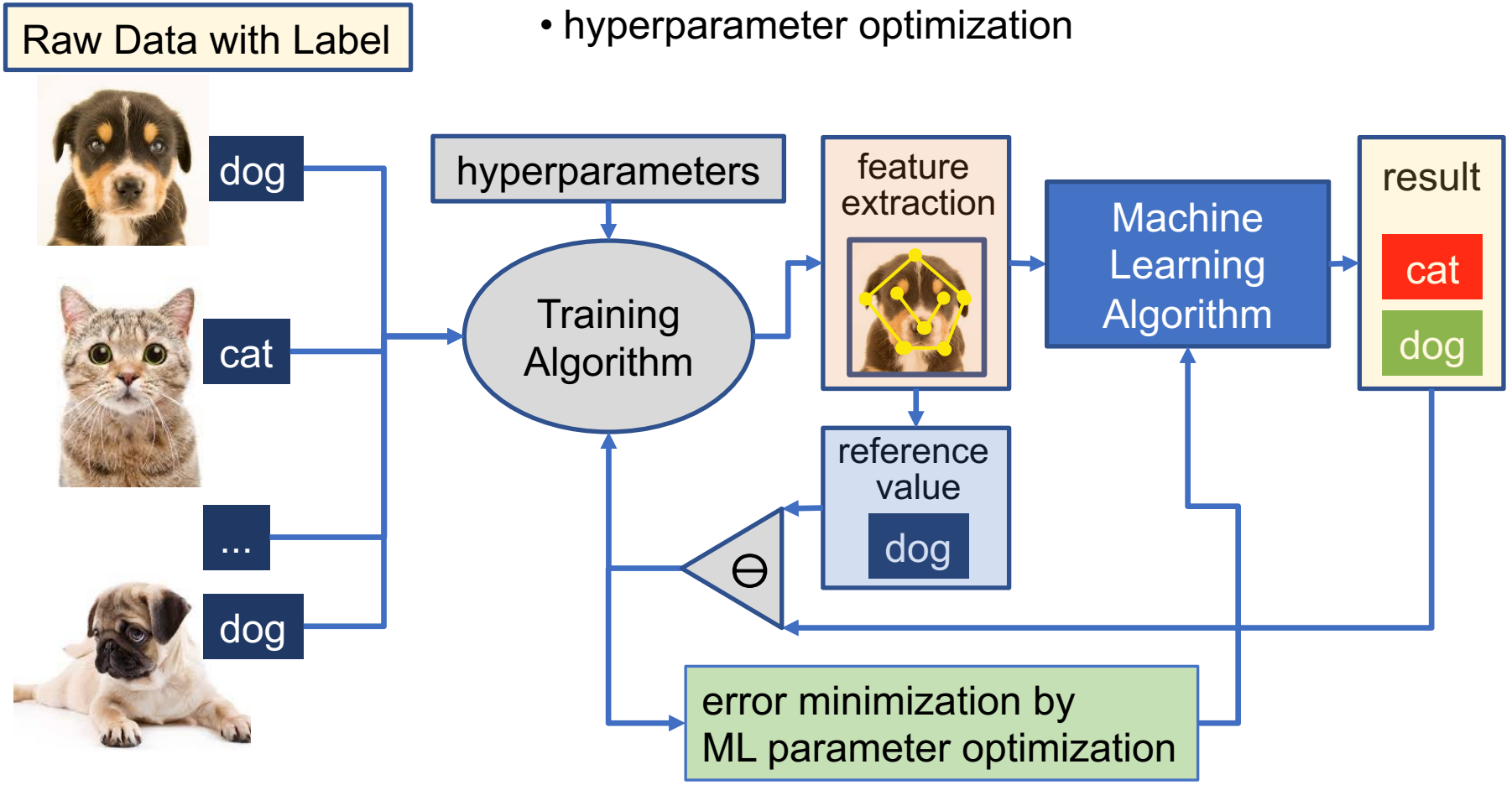
Supervised Learning: Classification

Task: Identify pictures of cats and dogs (classification)



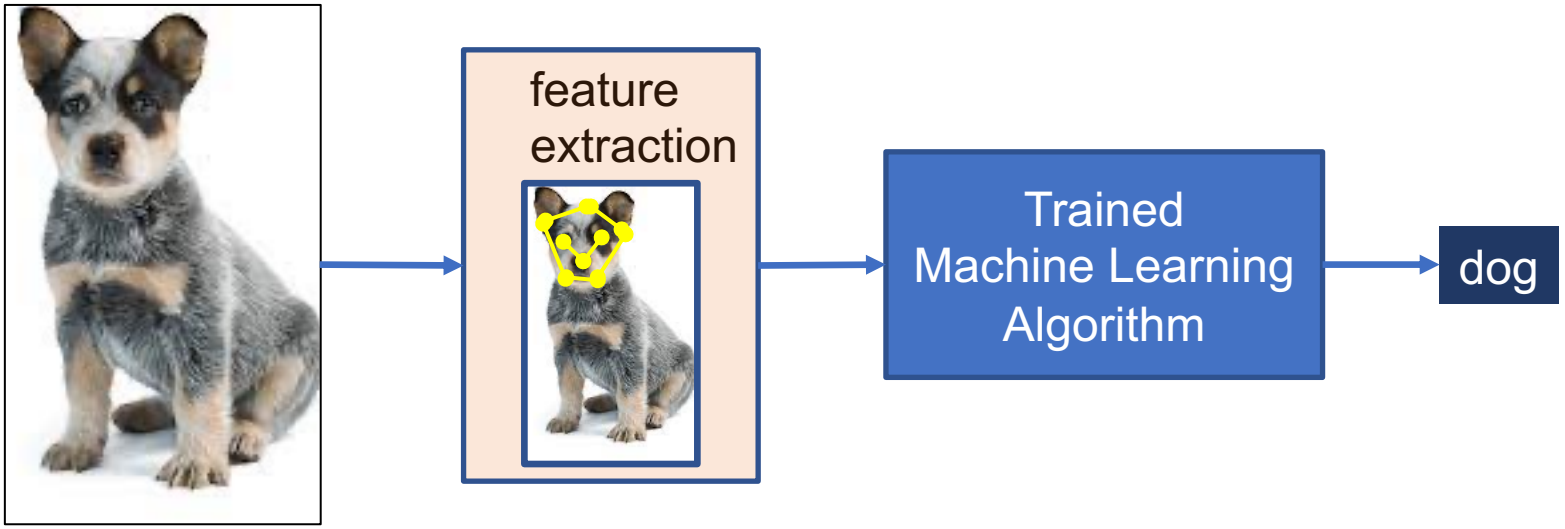
Supervised Learning: Training of ML Model

- choice of ML algorithm
- feature design
- hyperparameter optimization



Supervised Learning: Validation

Validation with unseen data



Supervised Learning: Feature Extraction

feature extraction

Automated feature extraction from raw data:

- convolutions of raw data (CNN)
- autoencoder
- Fast Fourier Transform
- N-point-statistics/auto correlation
- Principle Component Analysis
- Singular Value Decomposition

Feature extraction based on domain knowledge:

- extraction of physical quantities
- correlation analysis
- experience with similar tasks

Supervised Learning: Regression

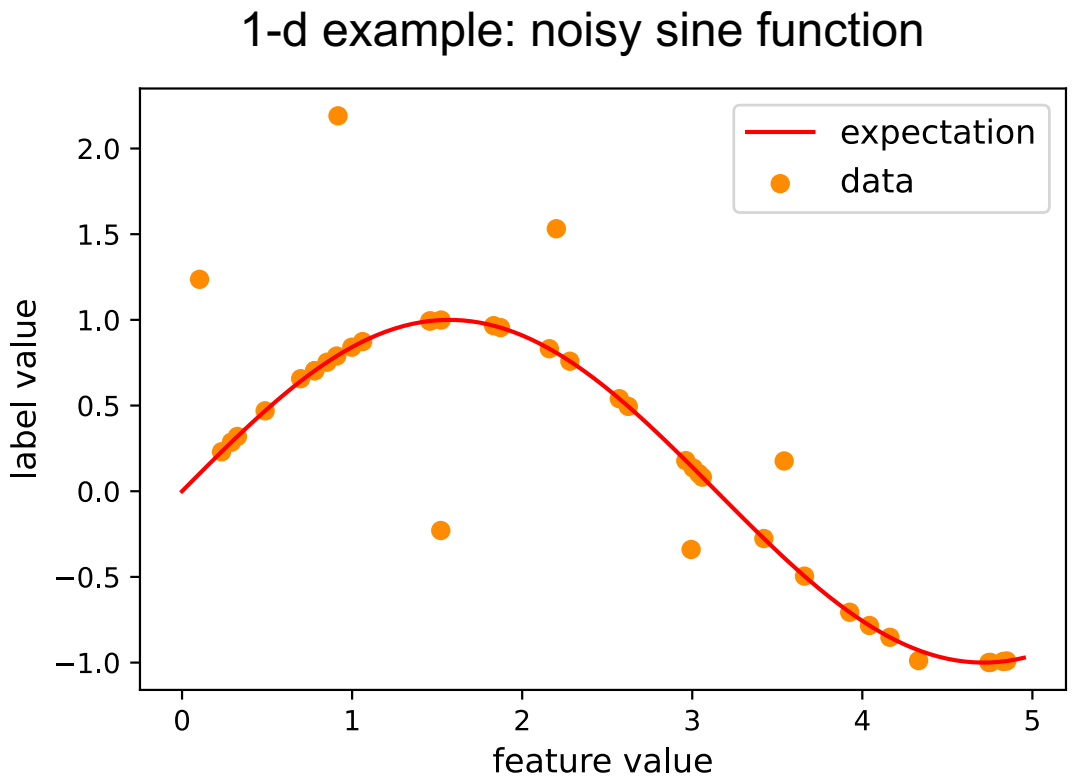
input vector "features"

Selection of features (or descriptors) determines the physics of the ML model

output vector "label" / result

Training Procedure
Find ML parameters that minimize deviation between result of ML model and known data point (ground truth).

Supervised Learning: Regression

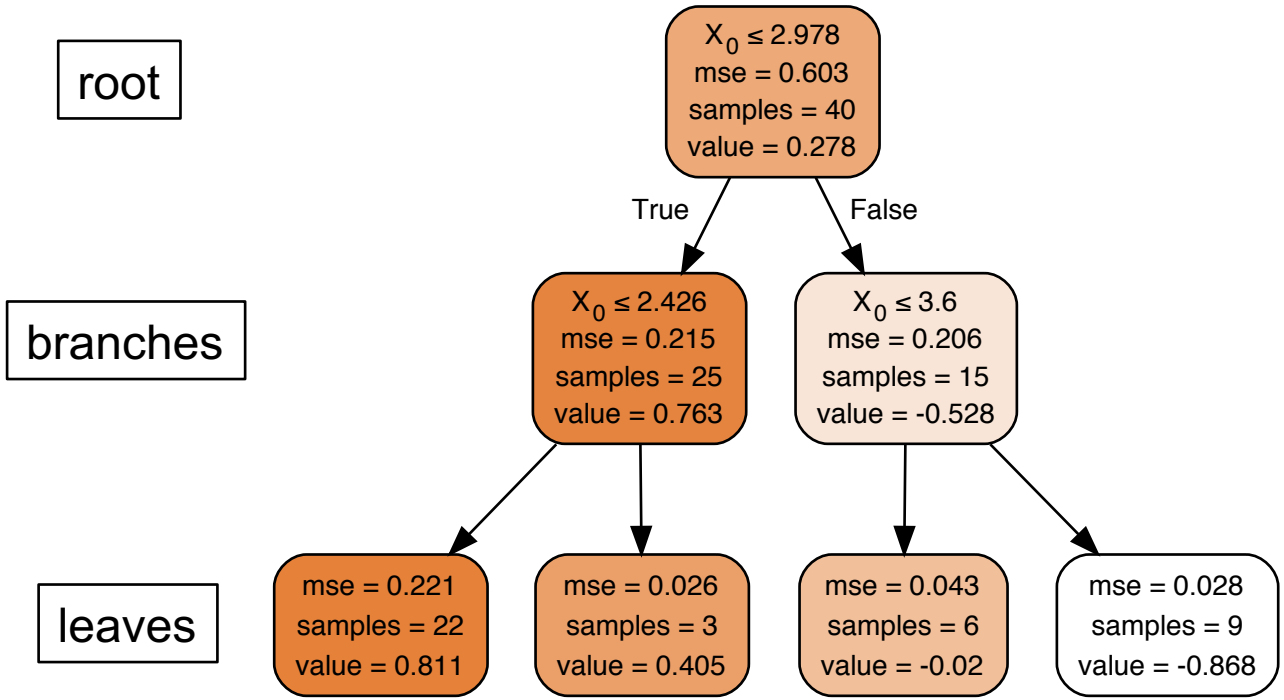


$$y = f(x) = \sin x$$

$$0 \leq x \leq 5$$

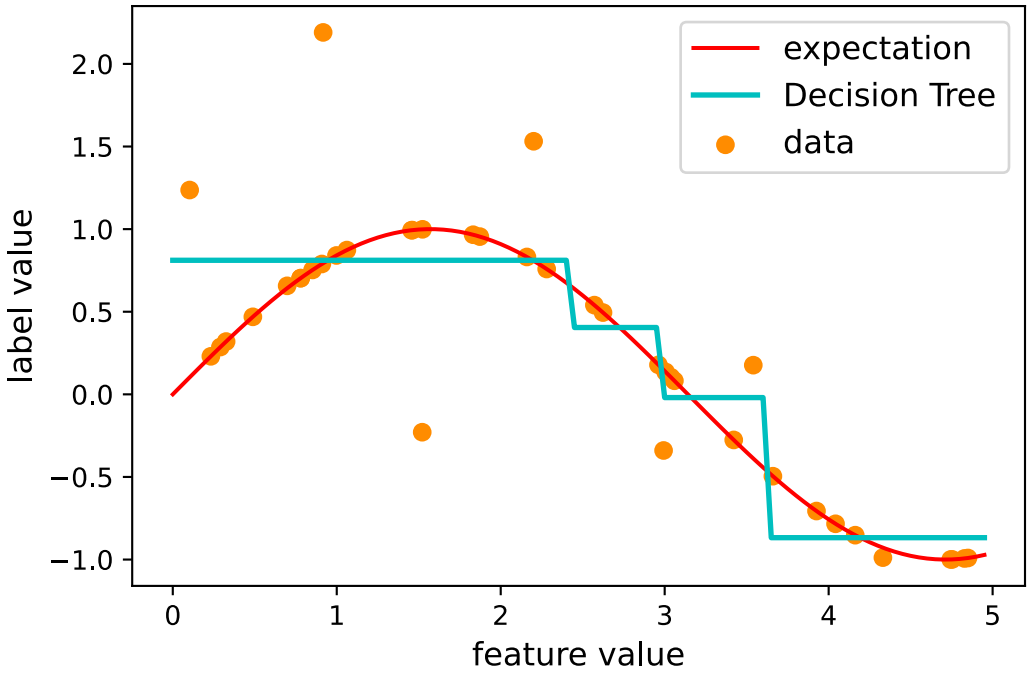
Decision Tree Regression

Succession of if-clauses leads to final result in “leaves”



Supervised Learning: Decision Tree Regression

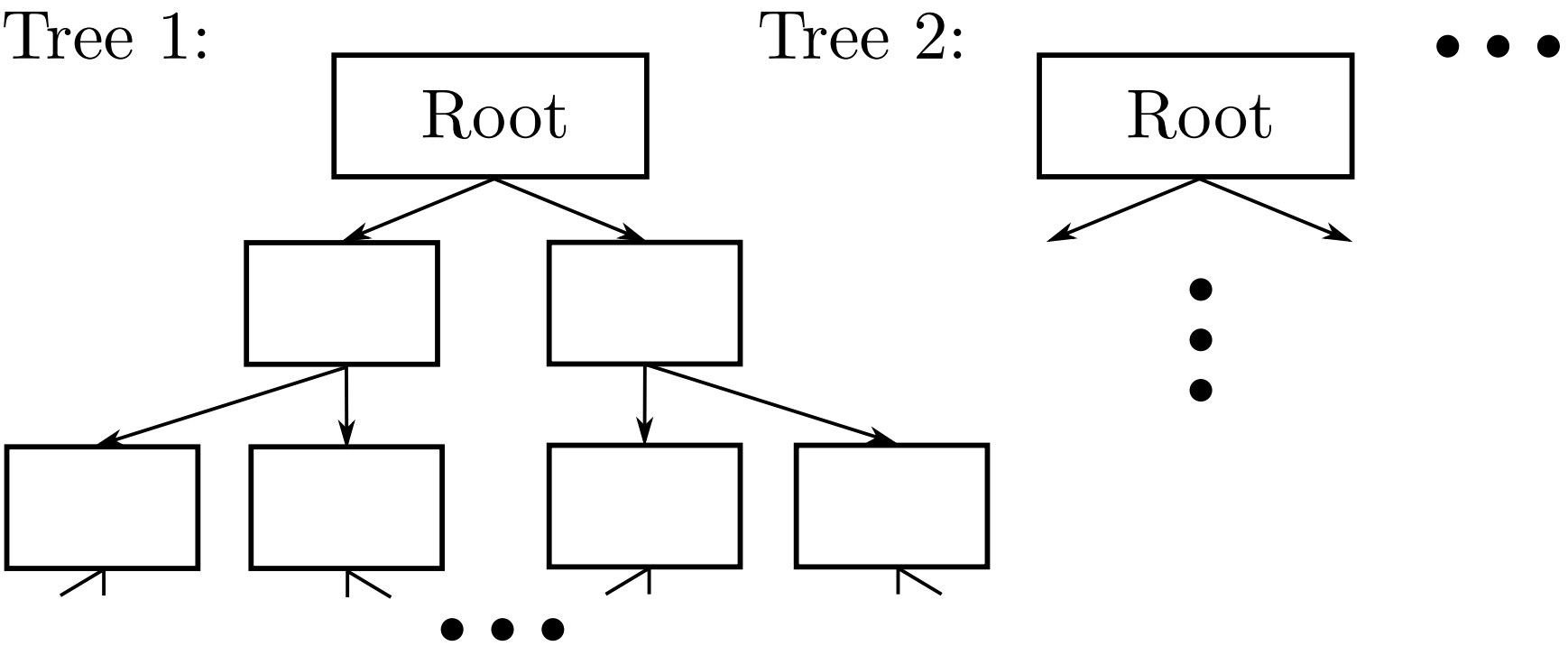
1-d example: noisy sine function



Decision Tree
hyperparameters:
depth = 2

$$y = f(x) = \begin{cases} 0.811 & \text{if} \quad x \leq 2.426 \\ 0.405 & \text{if} \quad 2.426 < x \leq 2.978 \\ -0.02 & \text{if} \quad 2.978 < x \leq 3.6 \\ -0.868 & \text{if} \quad x > 3.6 \end{cases}$$

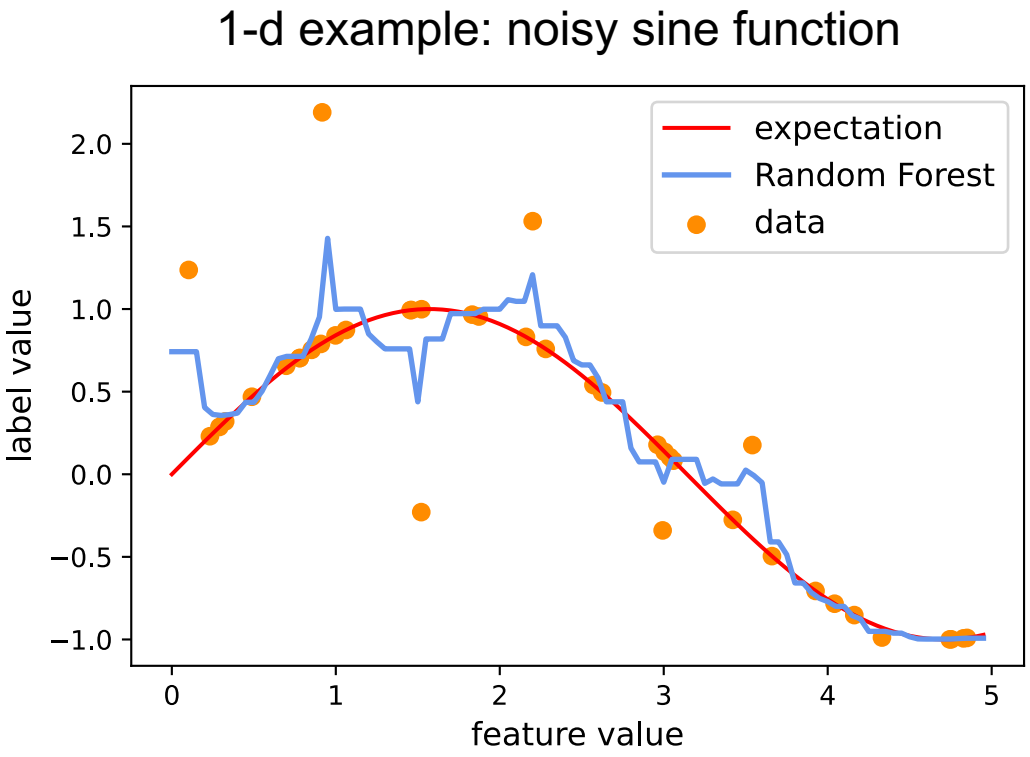
Random Forest Regression



Goal: Create model that predicts output value for given input data by learning simple decision rules

- Number of trees = 100 … 500
- Leaves contain either 1 or 0 samples
- Final result is average of the leave values obtained from all trees

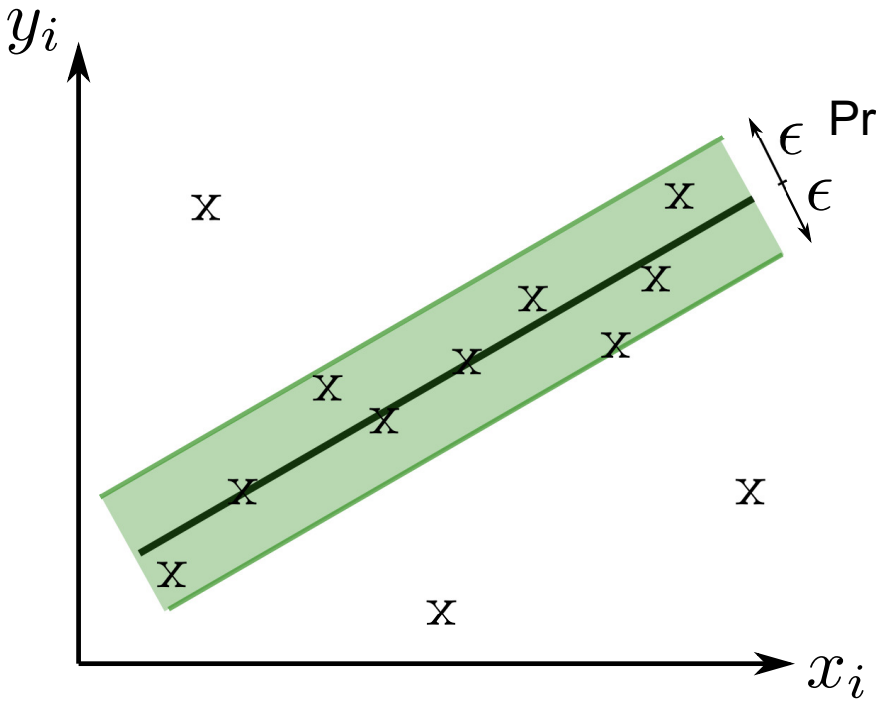
Supervised Learning: Random Forest Regression



Random Forest
hyperparameters:
max. depth = 5
N_{tree} = 20

$$y = f(x) = \frac{1}{N}\sum_{i=1}^{N} f_{DT}^{(i)}(x)$$

Support Vector Machine (Regression/Classification)



Precision ϵ = 1%

SVM function:

$$f(x) = \sum_{k=1}^{n} y_k a_k K\left(x_k^{(SV)}, x\right) + \rho$$

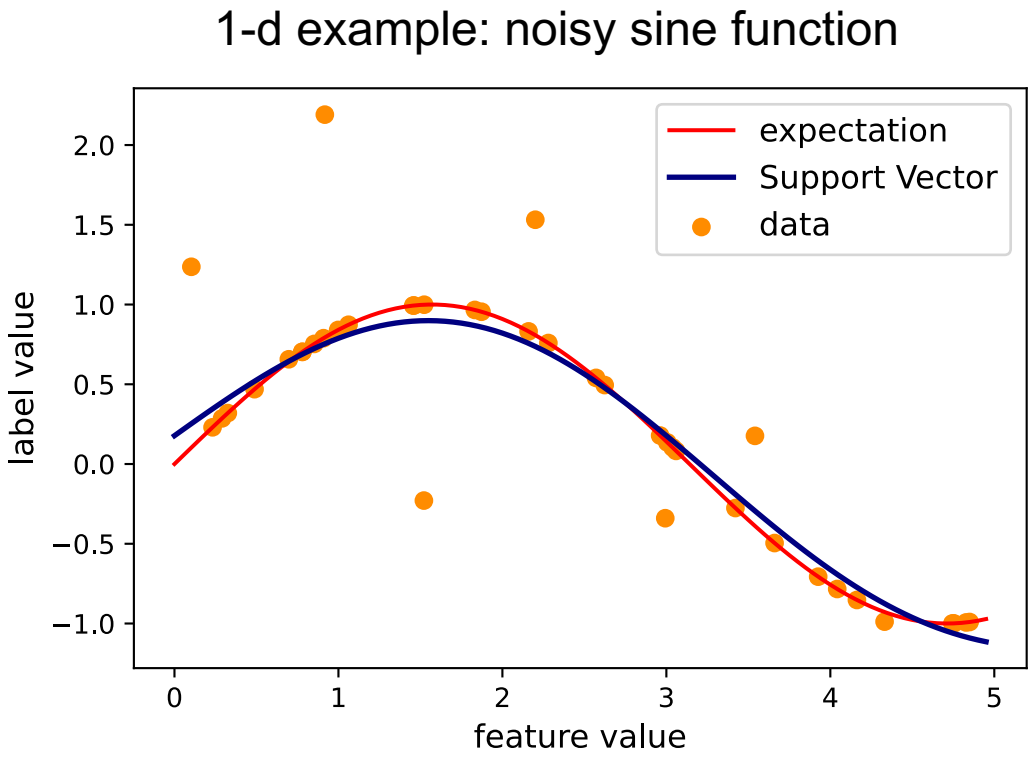
RBF kernel:

$$K\left(x_k^{(SV)}, x\right) = \exp\left(-\gamma \left\| x - x_k^{(SV)} \right\|^2\right)$$

Goal: Find a function such that data points lie within a corridor of $\pm\epsilon$ (function as flat as possible, actual error unimportant, penalty for outliers)

- Linear or Gaussian kernel for interpolation between support vectors
- Support vectors determined during training function (data points closest to target function)

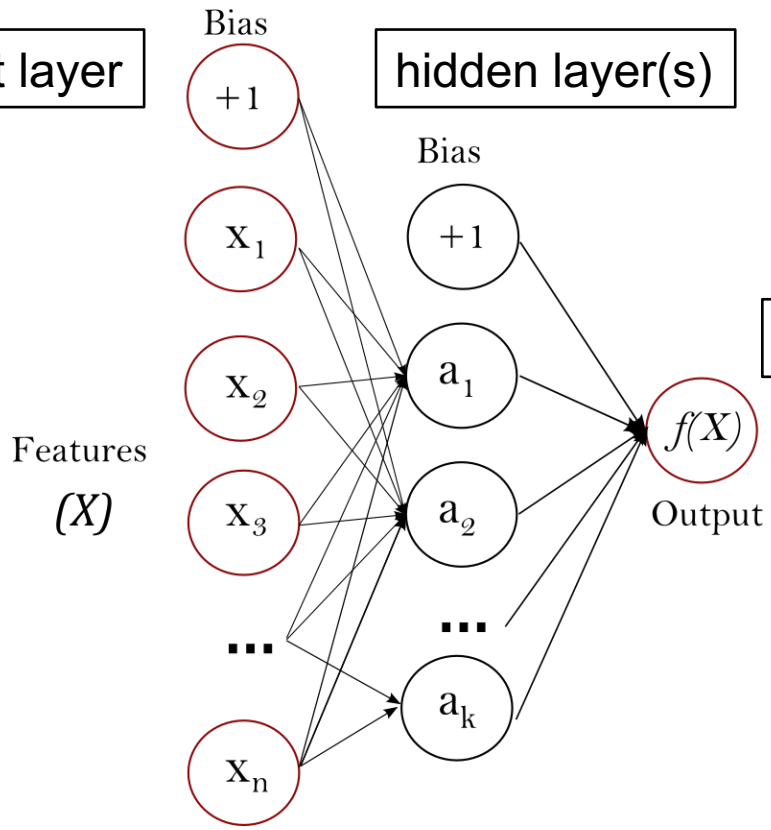
Supervised Learning: Support Vector Regression



Support Vector Mach.
hyperparameters:
C = 10
gamma = 0.1
kernel: radial basis fct.

$$f(x) = \sum_{k=1}^{n} y_k a_k K\left(x_k^{(SV)}, x\right) + \rho$$

Neural Networks (Regression/Classification)



$$f_{\text{neuron}}(x) = S(w \cdot x - U)$$

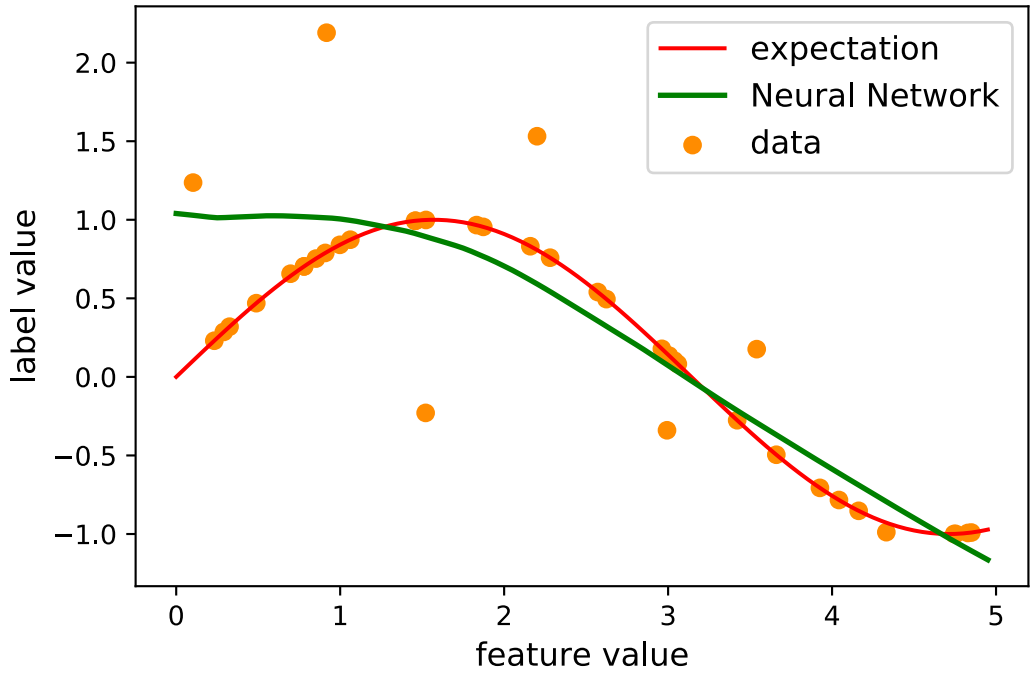
S: activation function (sigmoid, hyperb. tan, ...)
w: weight for input signals
U: bias

Goal: Find bias values and weights for activation functions that describe training data best. – *Deep learning*: multiple hidden layers.

Source: scikit-learn

Supervised Learning: Neural Network

1-d example: noisy sine function



Neural Network
hyperparameters:
hidden layers: 3
neurons: 100
activation function: relu
init. learning rate: 0.001
…

$$f(x) = \sum_{i=1}^{N_{\text{neuron}}} w^{(i)} f_{\text{neuron}}^{(i)}$$

Summary Machine Learning Methods

Common supervised Machine Learning (ML) methods

- Support Vector Machines
  (robust and moderate data requirements, only 2 hyperparameters)
- Neuronal Networks
  (prone to overfitting, large volumes of training data required, many hyperparameters)
- Gaussian Process
  (not covered here)
- Random Forrest
  (simple and robust reference method, prone to overfitting, only 2 hyperparameters)

Feature Selection determines physics of the trained model.

Hyperparameter tuning decisive for success of training.

Independent Validation necessary to ensure validity of trained model.

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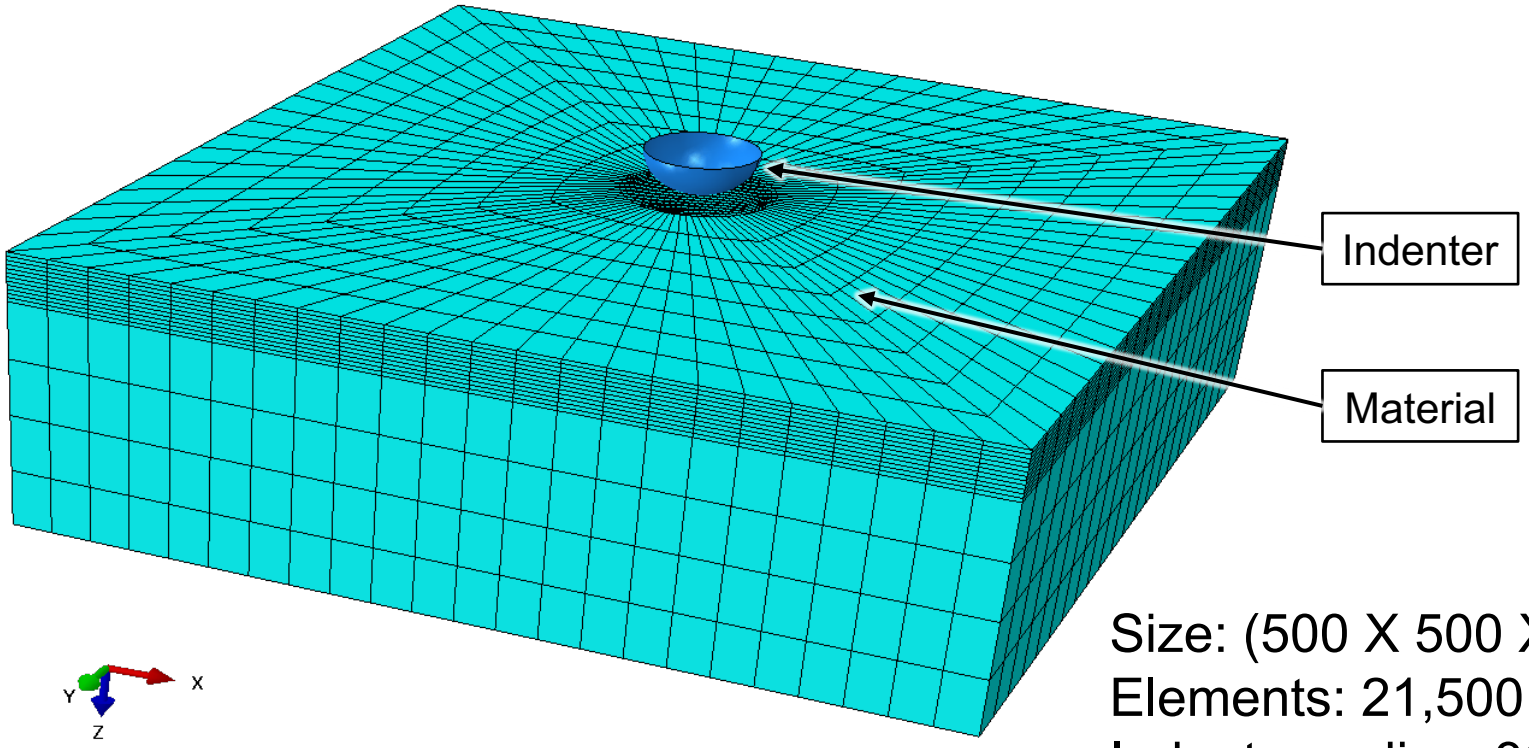
   2. ML-Regression

Finite Element Model of indentation

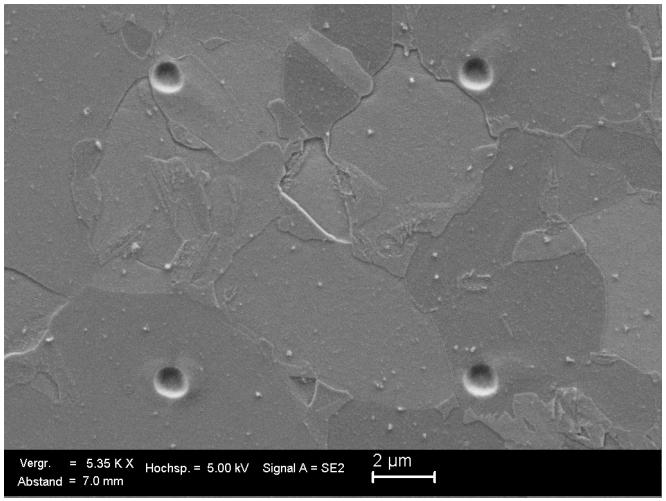


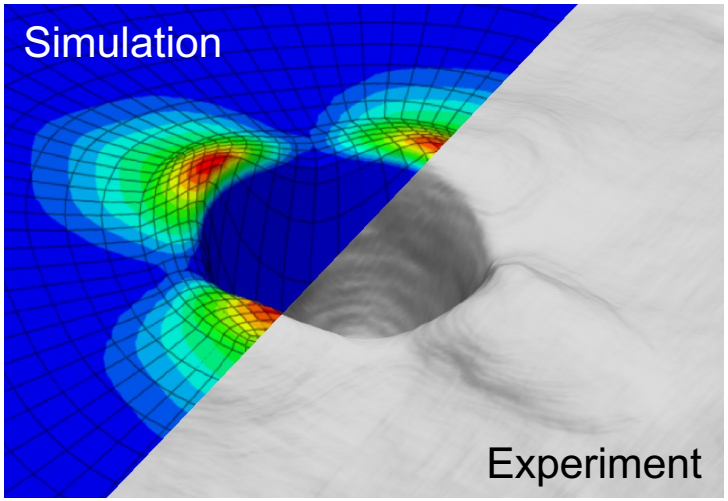
Size: (500 X 500 X 200) μm
Elements: 21,500
Indenter radius: 30 μm

- Finite element model gives accurate description of indentation process
- Simulation times hours to days, depending on model size and constitutive model

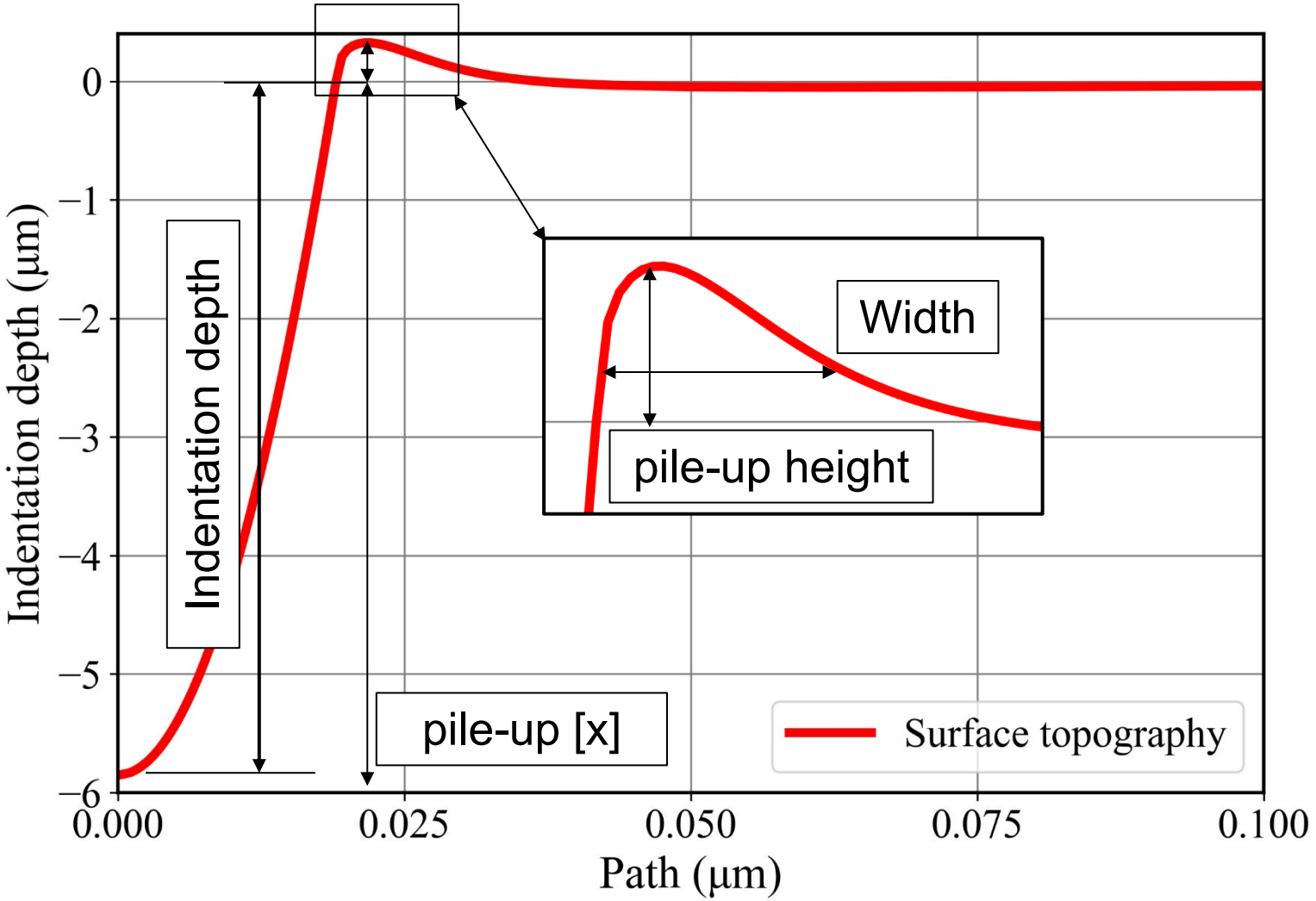
Finite Element Model of indentation

- Spherical nanoindentation into individual ferrite grains (ARMCO iron)
- Indenter tip radius: 800nm
- Max. load: 2.5 mN

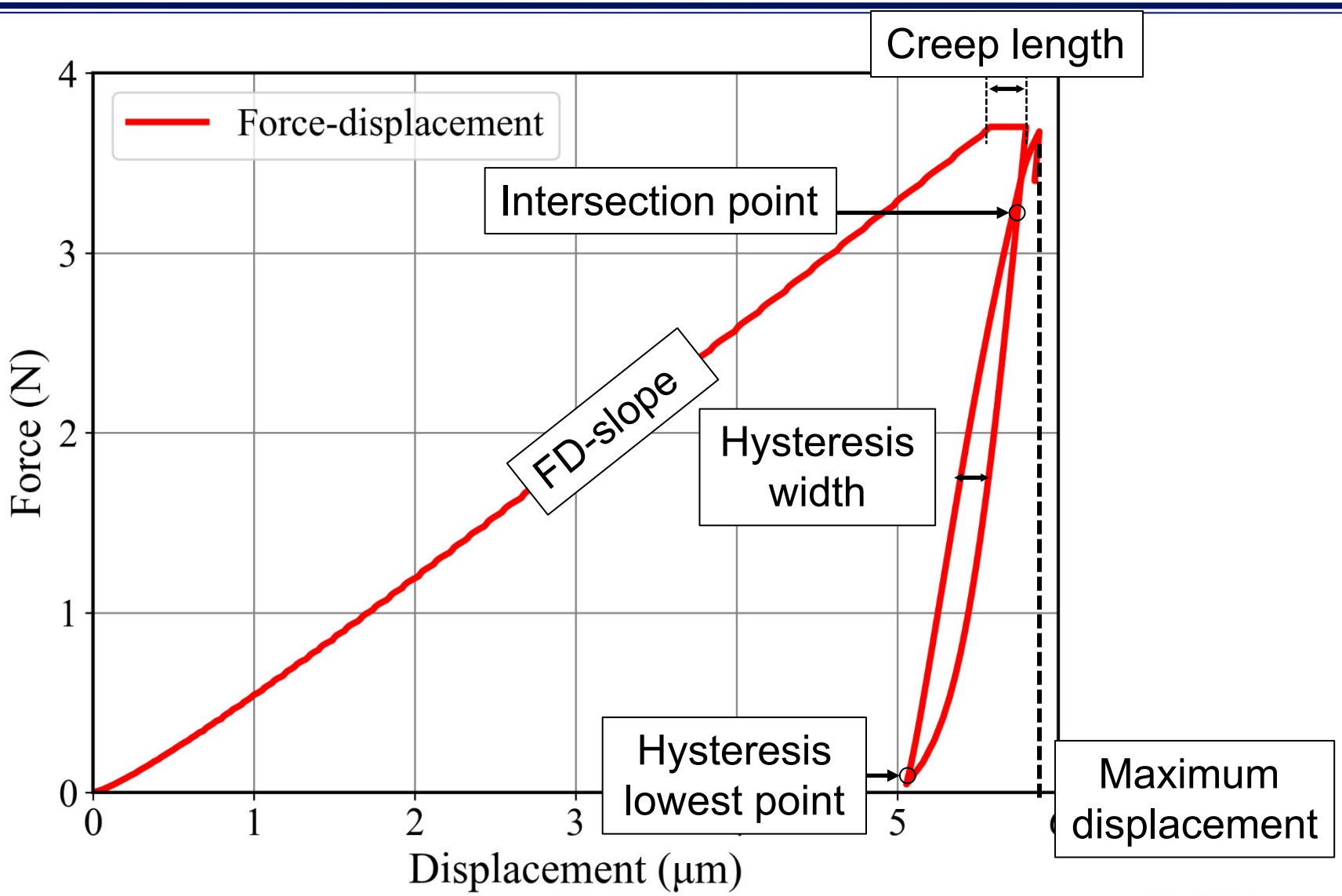




Definition of labels: Residual imprints



Definition of labels: Force-displacement curve



Data generation for training of ML surrogate model

Isotropic hardening

$$R = Q(1 - e^{-b\varepsilon_{eq}})$$

Non-linear kinematic hardening

$$\boldsymbol{\kappa} = \sum_{i}^{n} \boldsymbol{\kappa}_i ; d\boldsymbol{\kappa}_i = \frac{2}{3} C_i d\boldsymbol{\varepsilon}_p - g_i \boldsymbol{\kappa}_i d\varepsilon_{eq}$$

Creep/time-dependent deformation

$$\dot{\tilde{\varepsilon}}^{cr} = A\tilde{q}^n t^m = A_0 \left(\frac{q}{q_0}\right)^n \left(\frac{t}{t_0}\right)^m$$

1000 different combinations of material parameters are generated randomly from defined ranges.

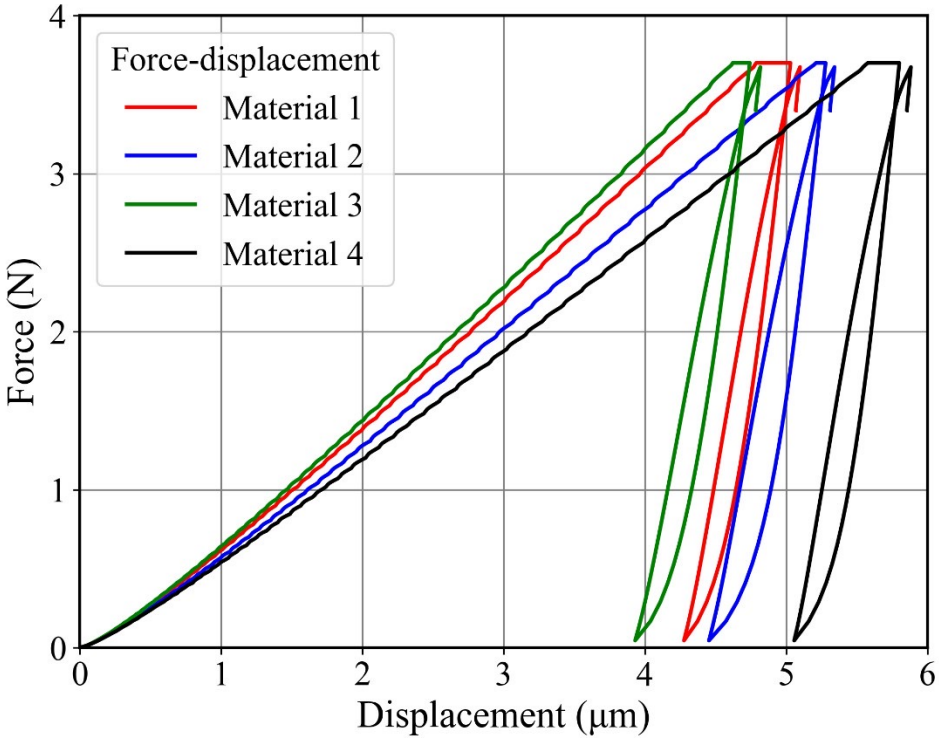
Material Parameter Ranges

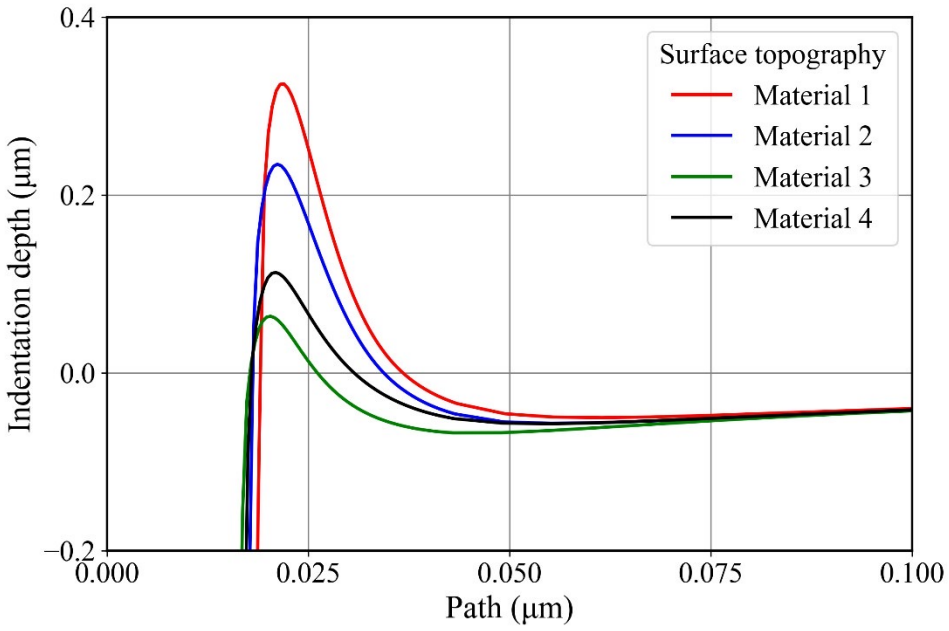
Parameter	Min	Max
A_0, 1/s	1E-07	1E-05
n, -	1.75	3.0
m, -	-0.95	-0.5
C_1, MPa	125000	225000
g_1, -	350	550
C_2, MPa	3000	5500
Q, MPa	-350	-1750
b, -	0.5	25

$$A = A_0 \, (750\text{MPa})^{-n} \, (100\text{s})^{-m}$$

Database generation

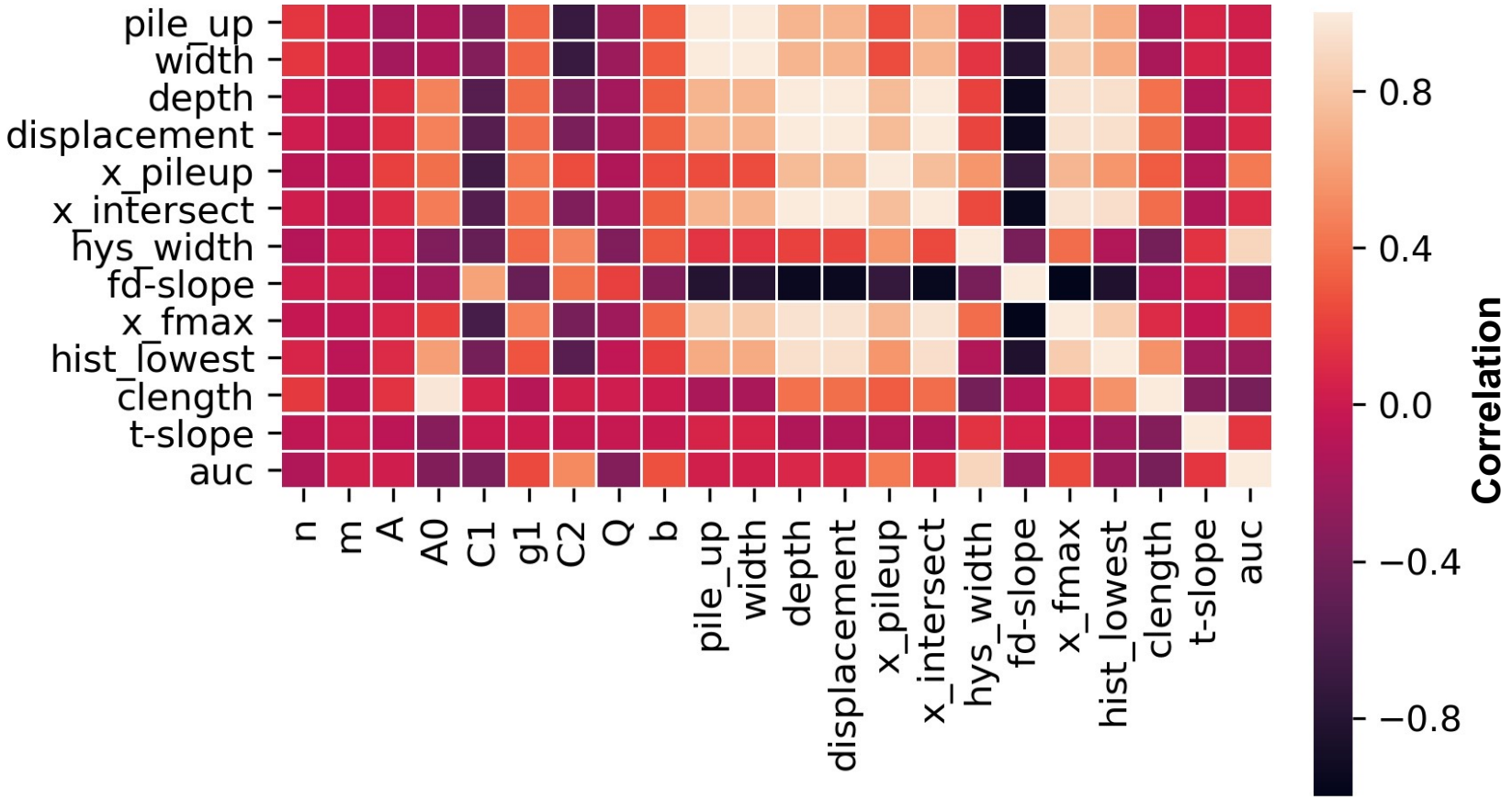
Simulation output





Feature selection

Heat map of extracted features and labels



Feature selection

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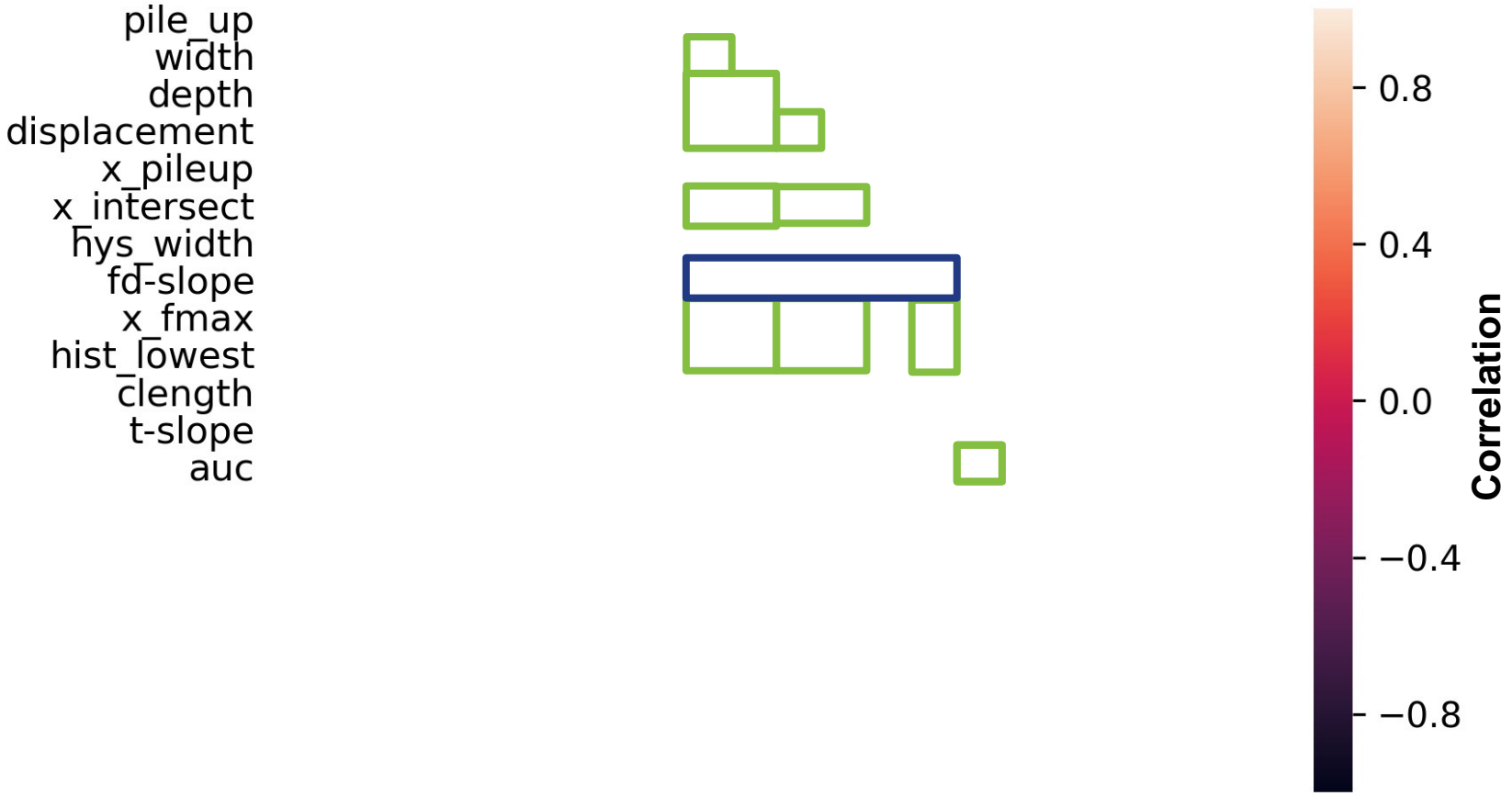
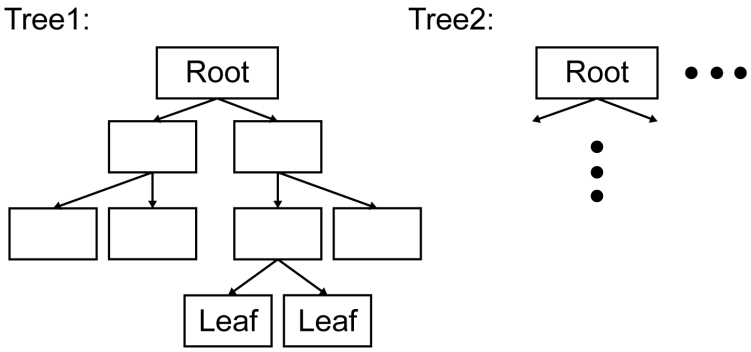
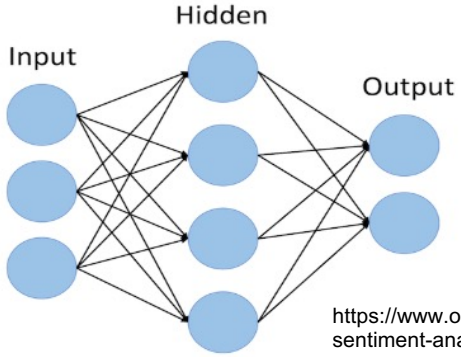


Training and testing of ML algorithms

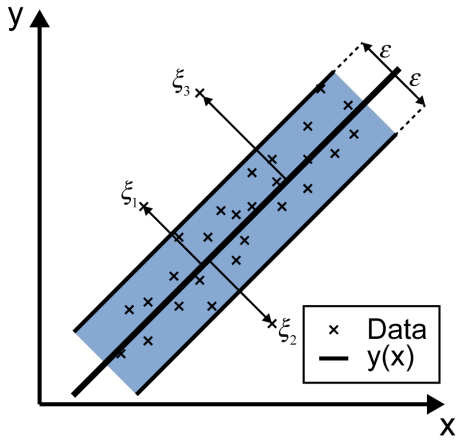


Random forest regression



https://www.oreilly.com/content/perform-sentiment-analysis-with-lstms-using-tensorflow/

Artificial neural networks

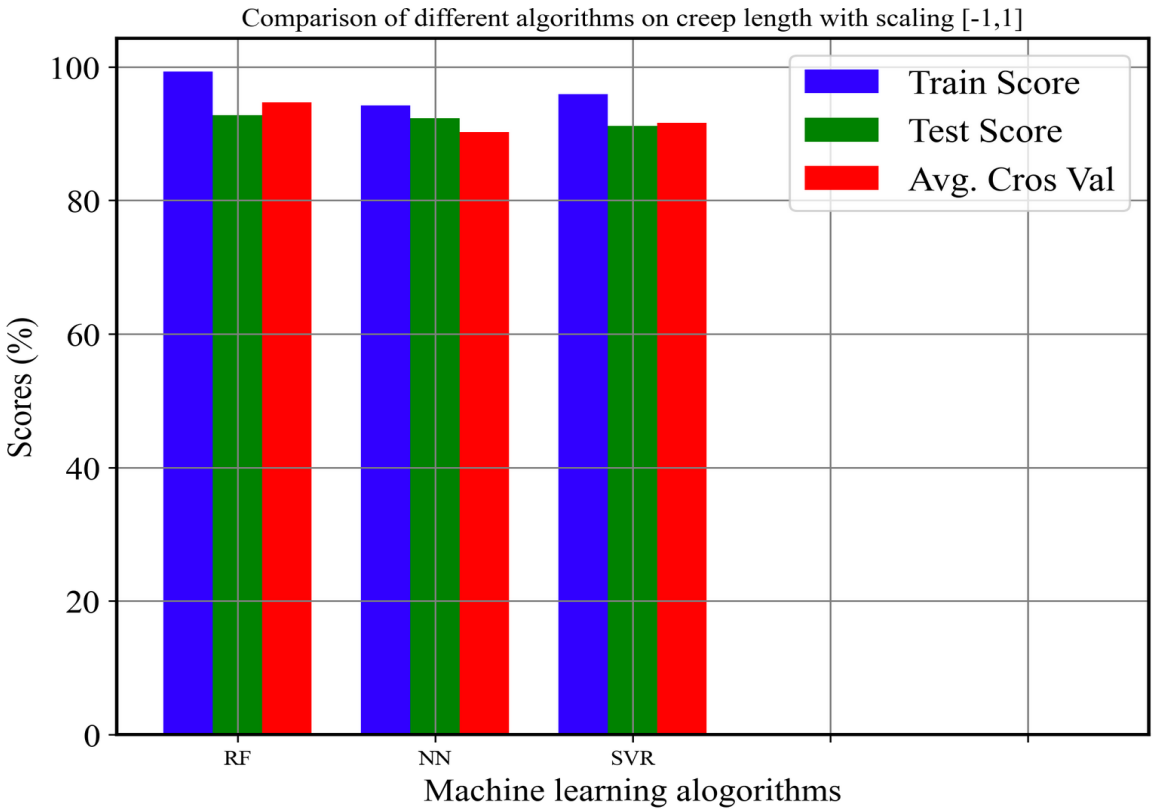


Support vector regression

- Machine learning library on Scikit Learn
- Random Forest Regression (RFR), Support Vector Regression (SVR), and Neural Networks (NN) are chosen.
- 75% training data and 25% testing data
- Grid search for determining hyperparameters

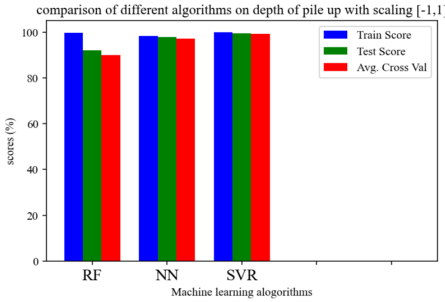
ML Regression for Characteristic Quantities

Function relating material parameters to characteristic quantities of indentation process:

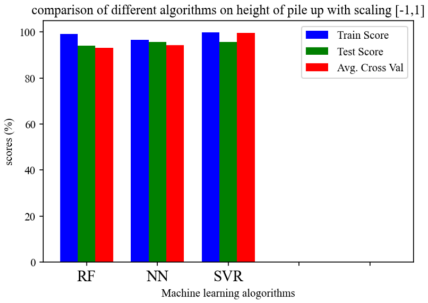


- creep length
- F-D slope
- indentation depth
- pile-up height
- …

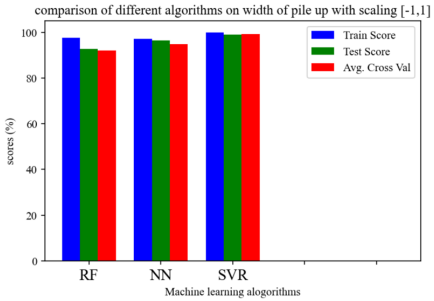
Training and testing results



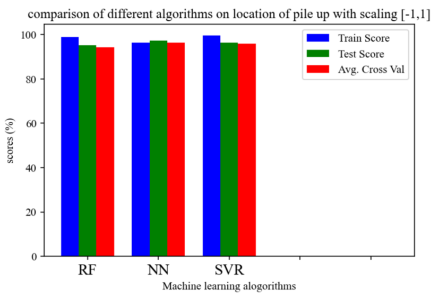
Indentation depth



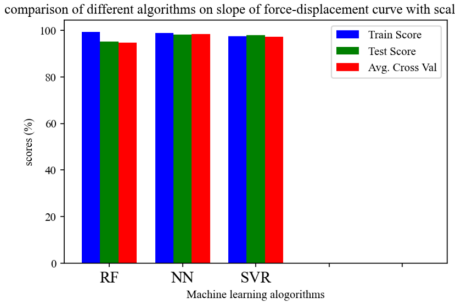
Pile-up height



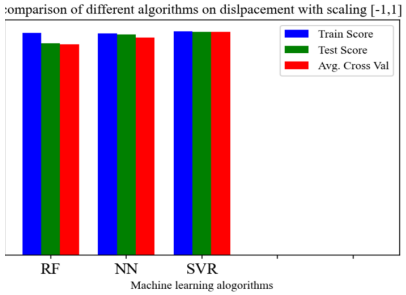
Pile-up width



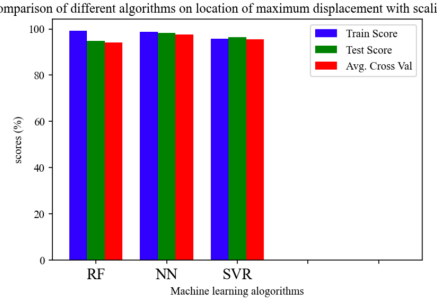
Pile-up location



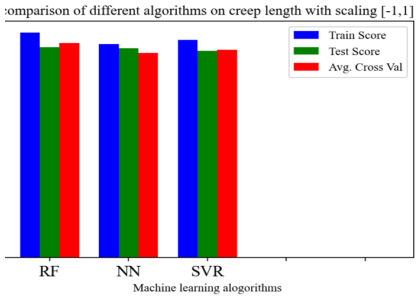
F-D slope



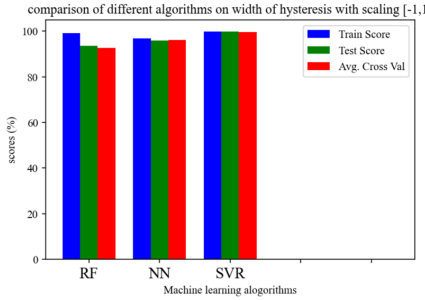
Displacement



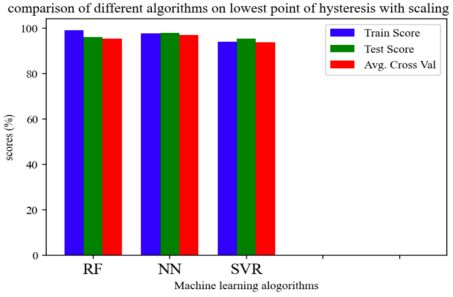
Max. displacement



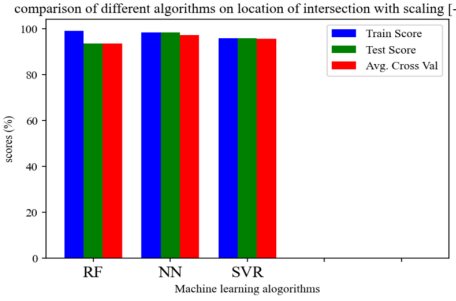
Creep length



Hysteresis width



Hyst. lowest point



Intersection point

Validation of surrogate model

	Pile up (µm)	x-pile up (µm)	Width (µm)	Depth (µm)	Displace-ment (µm)	X-intersect (µm)	Hys-width (µm)	Hys-lowest (µm)	Creep length (µm)	F-D slope (N/µm)
FEM	0.244	22.17	0.977	5.476	5.512	5.411	0.360	4.407	0.052	0.684
NN	0.230	22.22	0.953	5.568	5.576	5.572	0.353	4.686	0.062	0.676
NN Rel. dif. (%)	3.50%	0.23%	2.51%	1.68%	1.16%	2.97%	2.06%	6.32%	18.14%	1.28%
SVR	0.236	21.83	0.957	5.441	5.471	5.461	0.330	4.610	0.054	0.671
SVR Rel. dif. (%)	6.00%	1.52%	2.04%	0.64%	0.73%	0.91%	8.37%	4.60%	2.84%	1.96%
RFR	0.226	21.58	0.899	5.254	5.298	5.230	0.332	4.454	0.044	0.704
RFR Rel. dif. (%	7.53%	2.65%	8.04%	4.04%	3.87%	3.35%	7.82%	1.07%	14.26%	2.87%

Trained ML models are fed with unknown material parameters and compared with FEM simulation for validation

Relative difference:

$$\text{Rel. diff.} = \left| \frac{\text{FEM} - \text{predicted value}}{\text{FEM}} \right| * 100$$

Summary – Surrogate model

- Finite Element (FE) simulations can model mechanical problems with high accuracy
- For repeated tasks, as for example for inverse methods or optimization problems, the numerical cost of FE simulations poses a severe restriction
- Trained ML models can be used as numerically efficient surrogate models for such tasks – training effort only occurs once

Co-authors: H.M. Sajjad, Z. Hamzeh, P. Nooshmer, N. Vajragupta

unpublished work

Outline

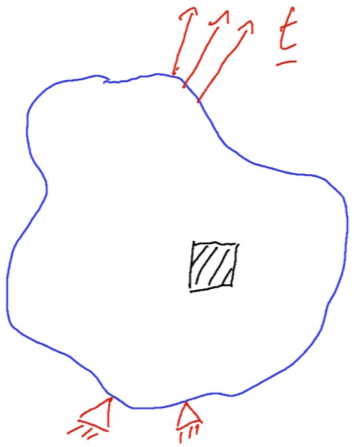
I. Lecture
   1. Machine Learning (ML) methods
   2. Applications as surrogate models for indentation
   3. Learning microstructure-property relationships

II. Tutorials
   1. ML-Classification
   2. ML-Regression

Constitutive modeling (State-of-the-Art)

Component
Mechanical / thermal / environmental loading conditions

total strain rate $\dot{\boldsymbol{\varepsilon}}_{\mathrm{tot}}$
temperature T
deformation history $\boldsymbol{\varepsilon}_{\mathrm{pl}}$



Constitutive models
History dependent evolution equations for state variables

$$\dot{\boldsymbol{\sigma}} = \dot{\boldsymbol{\sigma}}\left(\boldsymbol{\sigma}, \boldsymbol{\varepsilon}_{\mathrm{pl}}, \dot{\boldsymbol{\varepsilon}}_{\mathrm{tot}}, D, T\right)$$
$$\dot{\boldsymbol{\varepsilon}}_{\mathrm{pl}} = \dot{\boldsymbol{\varepsilon}}_{\mathrm{pl}}\left(\boldsymbol{\sigma}, \boldsymbol{\varepsilon}_{\mathrm{pl}}, \dot{\boldsymbol{\varepsilon}}_{\mathrm{tot}}, D, T\right)$$
$$\dot{D} = \dot{D}\left(\boldsymbol{\sigma}, \boldsymbol{\varepsilon}_{\mathrm{pl}}, \dot{\boldsymbol{\varepsilon}}_{\mathrm{tot}}, D, T\right)$$

Material parameters
Material specific input to constitutive models

elastic tensor C_{ijkl}
yield strength σ_y
work hardening rate $\partial\boldsymbol{\sigma}/\partial\boldsymbol{\varepsilon}_{\mathrm{pl}}$
damage onset $\varepsilon_{\mathrm{pl}}^{\mathrm{crit}}$

Material response
Time dependent state variables

stress tensor $\boldsymbol{\sigma} = \boldsymbol{\sigma}(t)$
plastic strain $\boldsymbol{\varepsilon}_{\mathrm{pl}} = \boldsymbol{\varepsilon}_{\mathrm{pl}}(\mathrm{t})$
damage $D = D(t)$

Problem
- Solutions involve rather intricate mathematical formalism
- Explicit consideration of microstructure is difficult
- Material parameters vary with microstructure

Constitutive Modeling: Digital Twin of Material

Component
Mechanical / thermal / environmental loading conditions

total strain rate $\dot{\boldsymbol{\varepsilon}}_{\mathrm{tot}}$
temperature T
deformation history $\boldsymbol{\varepsilon}_{\mathrm{pl}}$

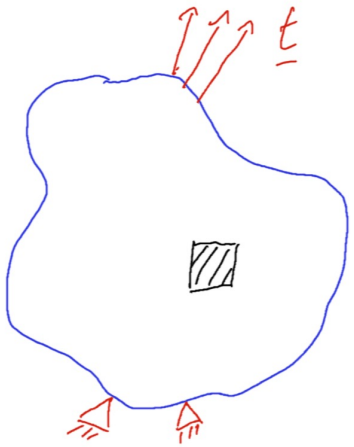
Digital Twin

Data-based material representation

- mechanical & functional properties
- transport properties
- explicit consideration of microstructure

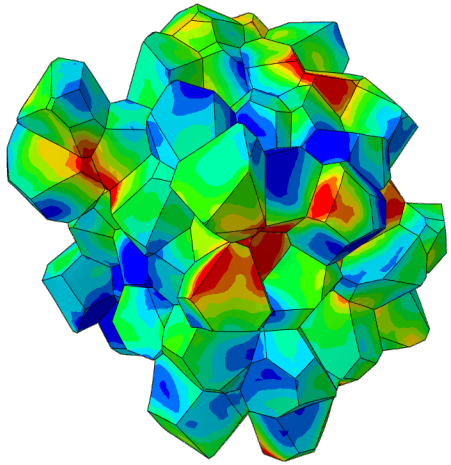
Material response
Time dependent state variables

stress tensor $\boldsymbol{\sigma} = \boldsymbol{\sigma}(t)$
plastic strain $\boldsymbol{\varepsilon}_{\mathrm{pl}} = \boldsymbol{\varepsilon}_{\mathrm{pl}}(\mathrm{t})$
damage $D = D(t)$

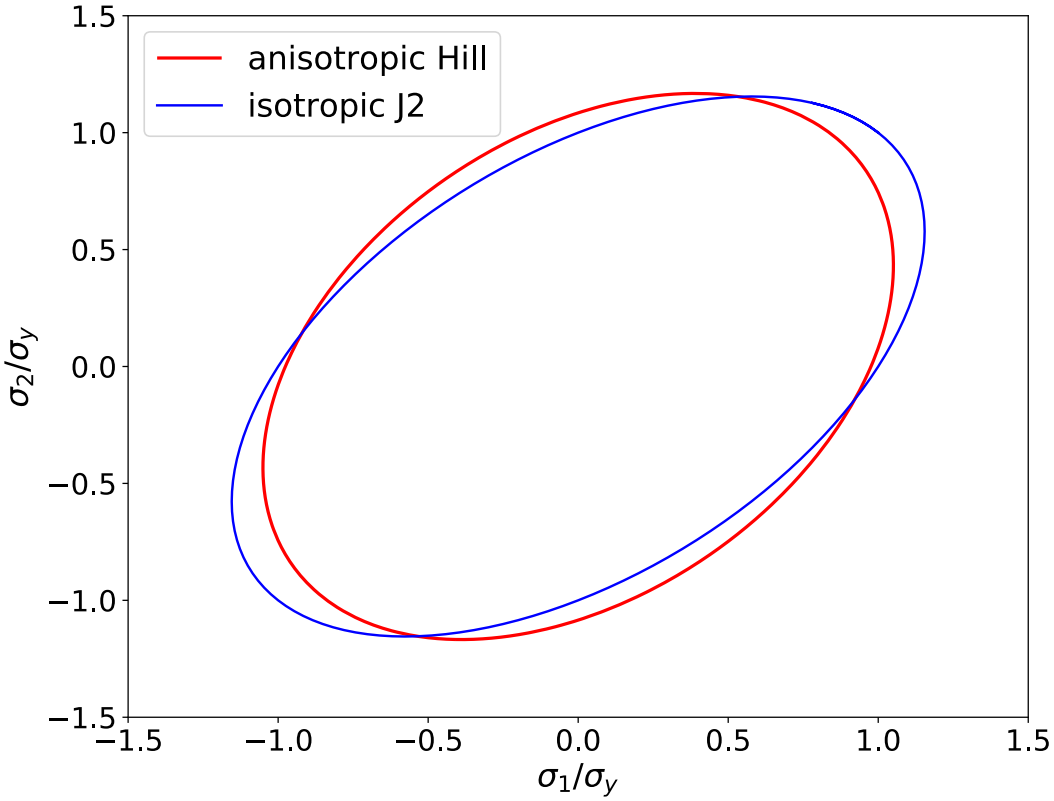


Hybrid materials data

- physics-based models
- experiment



Continuum plasticity



Yield loci of isotropic J2 and anisotropic Hill material definitions in cross-section of principle stress space

Yield function

$$f(\boldsymbol{\sigma}) = \sigma_{\mathrm{eq}} - \sigma_y$$

Yield locus $f(\boldsymbol{\sigma}) = 0$

- elasticity inside $f(\boldsymbol{\sigma}) < 0$
- plasticity on yield locus
- material does not support stresses outside yield locus

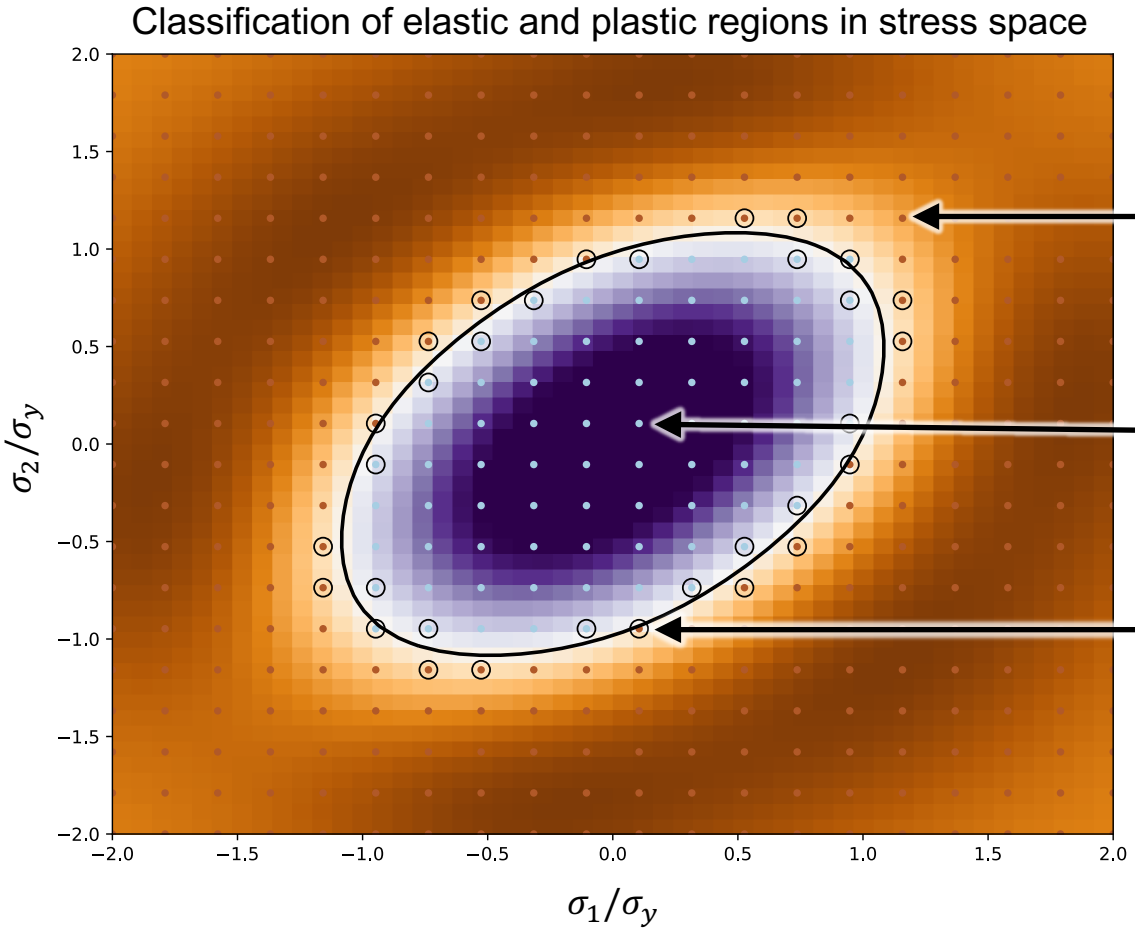
Plastic strain rate (flow rule)

$$\dot{\boldsymbol{\varepsilon}}_{\mathrm{pl}} = \dot{\lambda}\boldsymbol{n}$$

- $\dot{\lambda}$: plastic strain multiplier obtained from return mapping algorithm
- $\boldsymbol{n}$: normal to yield locus

Data-based model for plastic yielding

Trained Support Vector Classification



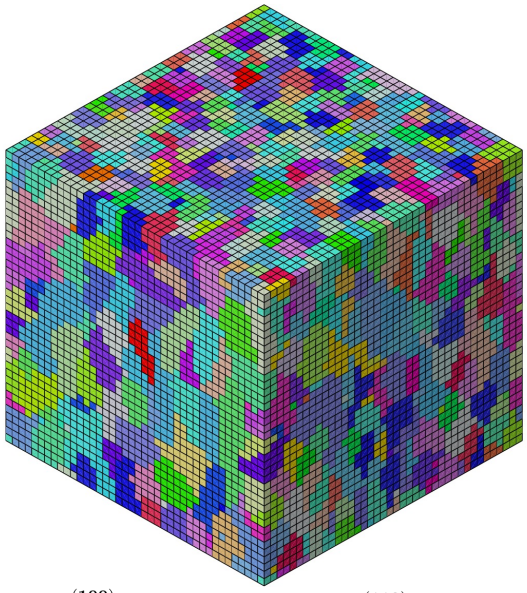
Data points (stresses) classified as “plastic” ($f \geq 0$)

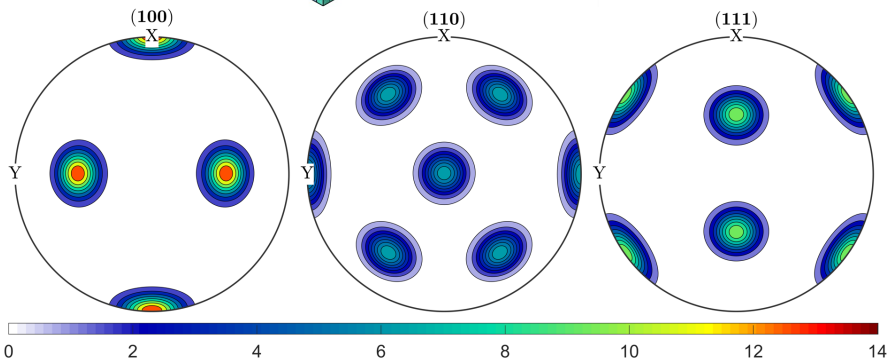
Data points (stresses) classified as “elastic” ($f < 0$)

Support vectors (data points close to delimiter)

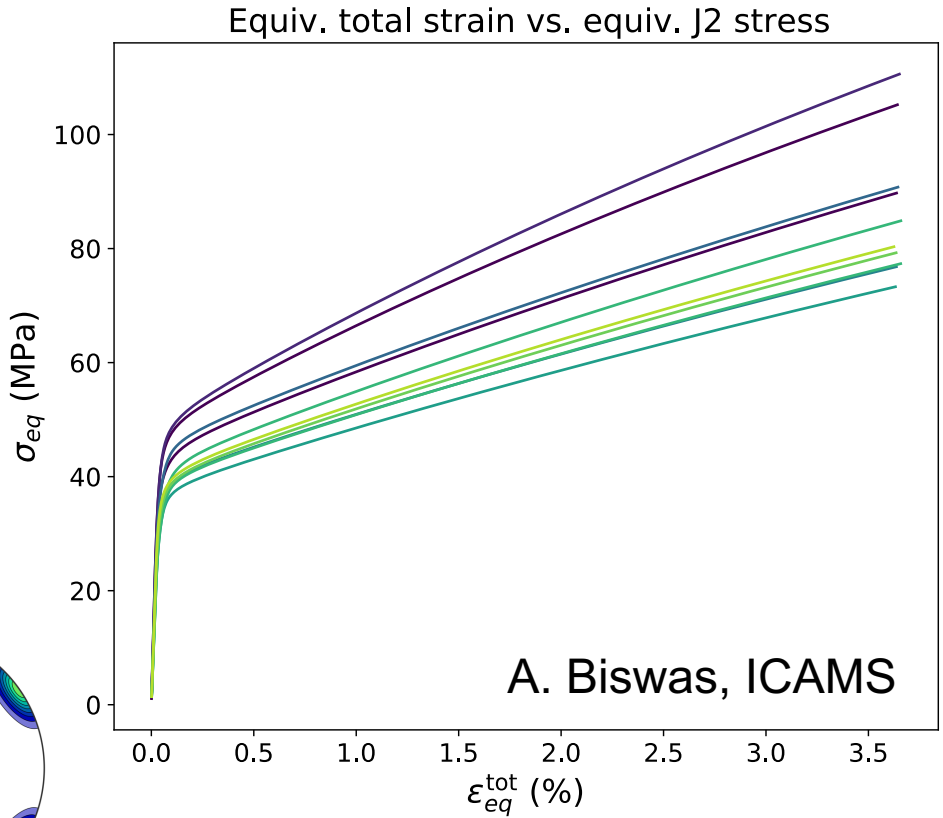
A. Hartmaier Materials 2020

Training Data Generation by Micromechanical Model





Micromechanical model with ~2,200 grains and Goss texture

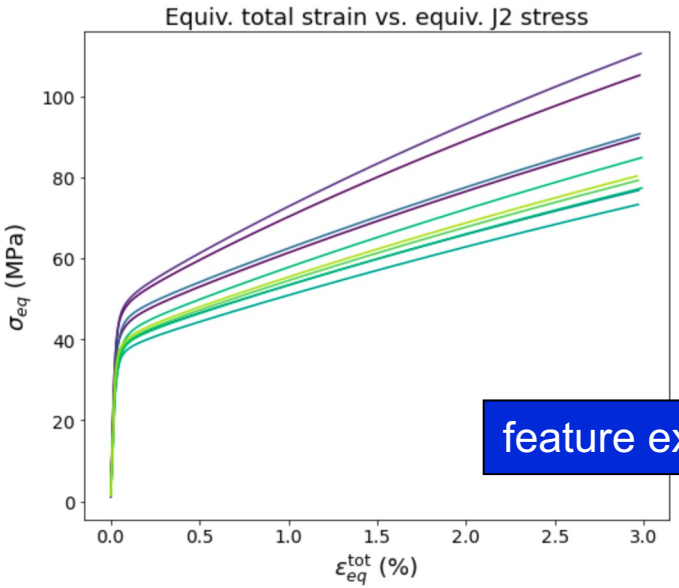


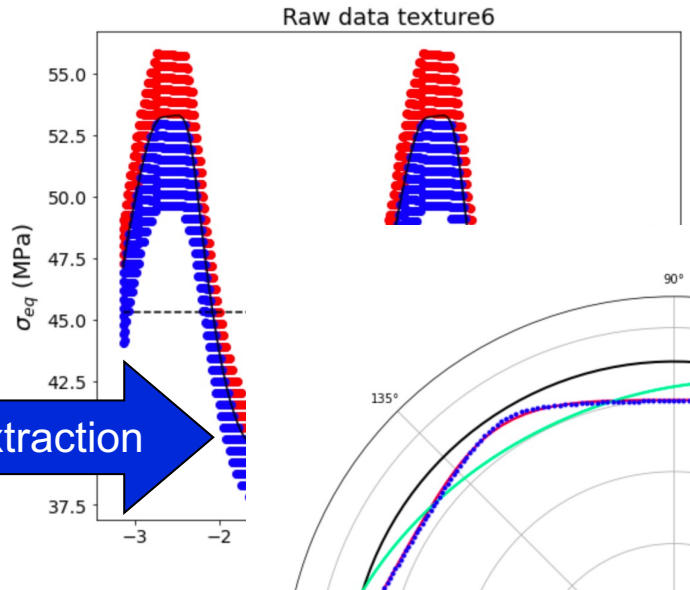
Resulting stress-strain curves

- Crystal plasticity model
- Different deviatoric load cases

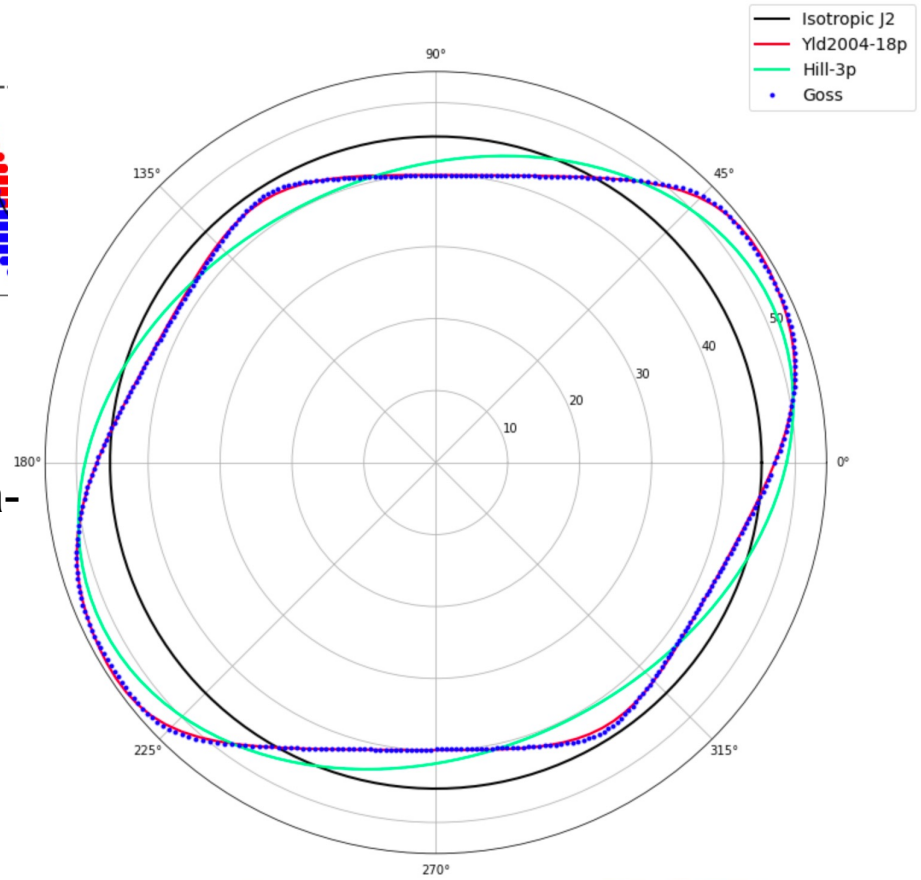
Anisotropic yield strength → data

Training of Classifier for Elastic / Plastic Regions





feature extraction

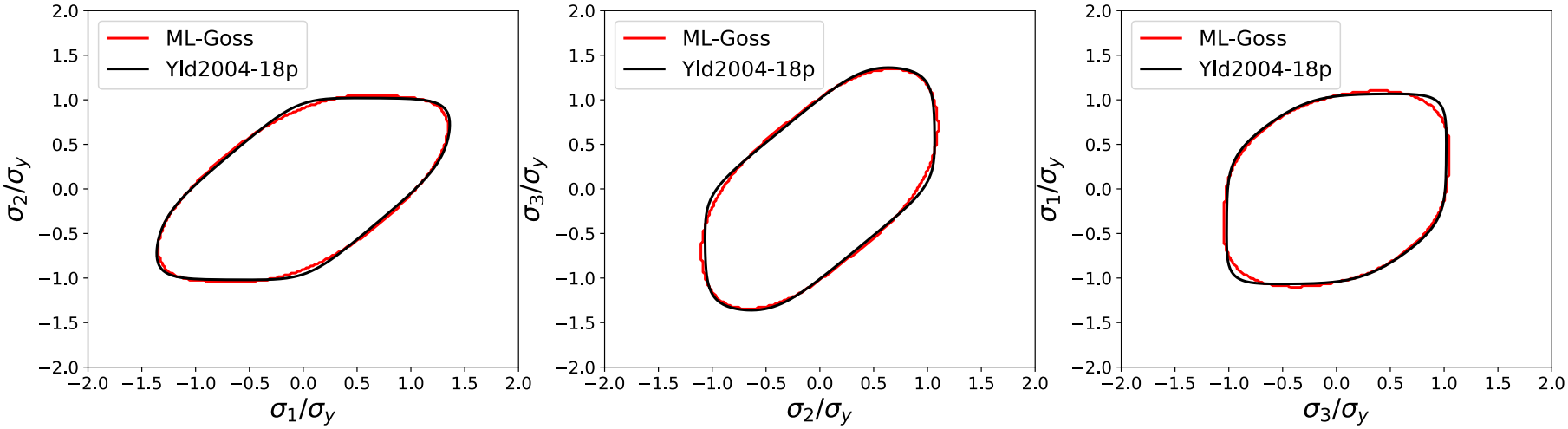


Digital Twin: Microstructure sensitive data-based description of plastic material properties

Experimental data

- validation of micromechanical model
- hybrid mechanical data bases

Trained Machine Learning Flow Rule

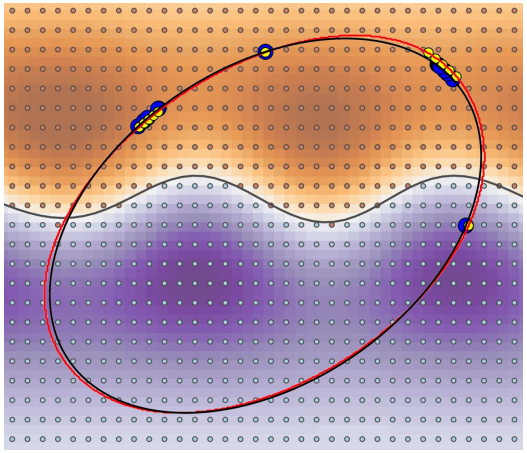


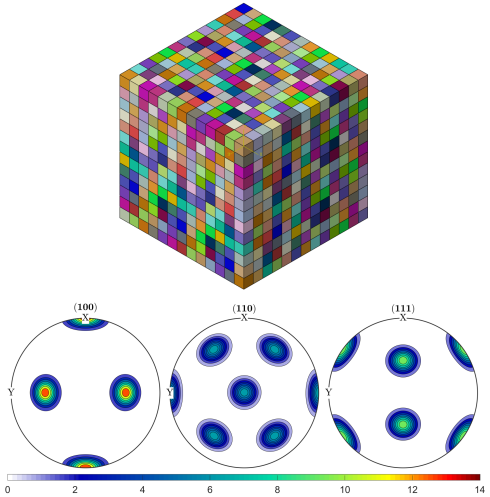
Yield loci in different cross-sections of principle stress space

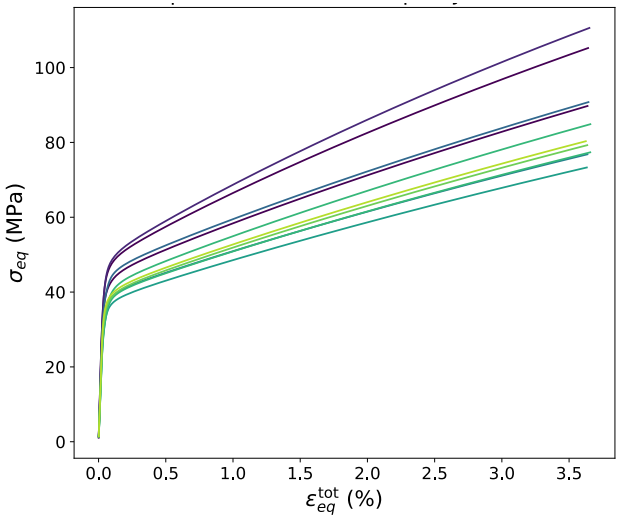
- Mechanical data obtained from micromechanical model
- Training of Machine Learning flow rule
- Barlat Yld2004-18p yield function fitted to same data

Summary

- **Data-oriented material descriptions based on ML models** can replace classical constitutive rules and their parameters in finite element modeling
  → Advantage: **Explicit consideration of microstructure** is possible
- Micromechanical modeling (synthetic RVEs, crystal plasticity, damage) is a powerful tool to generate **data for microstructure-property relationships**
- Fully parameterized and validated micromechanical models can complement experimental data to **hybrid mechanical data**







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   Use tutorials on MyBinder.org launch binder

   Installation from GitLab repository:
   https://gitlab.ruhr-uni-bochum.de/hartmajg/ml-tutorial.git