Using machine learning algorithms to interpret finite element simulations of indentation experiments including tip radii effects

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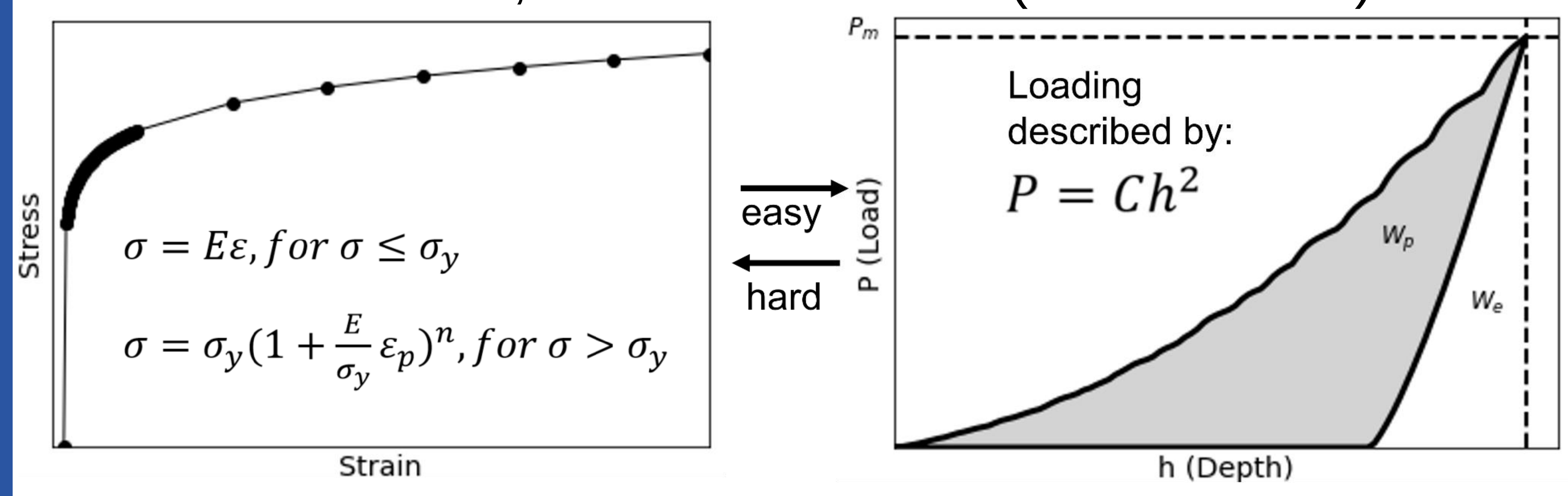
Motivation:

- Nanoindentation is a common, nearly non-destructive technique for **fast evaluation of materials properties.**
- There are numerous approaches for data evaluation. The technique has issues with scaling from local to global parameters**, tip radius effects, substrate influence.** The inverse calculation especially of plastic parameters is usually performed with fitting functions (high errors) or co-simulation (high time consumption).
- For this poster 2D (minutes calculation time) and 3D Simulations (hours) were used to calculate parameters once in the **parameter space of metals.**

Simulations:

185 2D Simulations, 58 3D Simulations (20% Test Set)



Abaqus-Python Models used to loop materials parameters of metals and tip-radii. Indentation depth assumed as constant for all simulations. Material Model implemented as Fortran subroutine by [1].

Features:

9 Features were extracted from the indentation curve:

Unloading slope	Loading Curvature	Normalized Curvature*
Normalized Slope*	Elastic Work	Plastic Work
h ratio	Work Ratio	Total Work

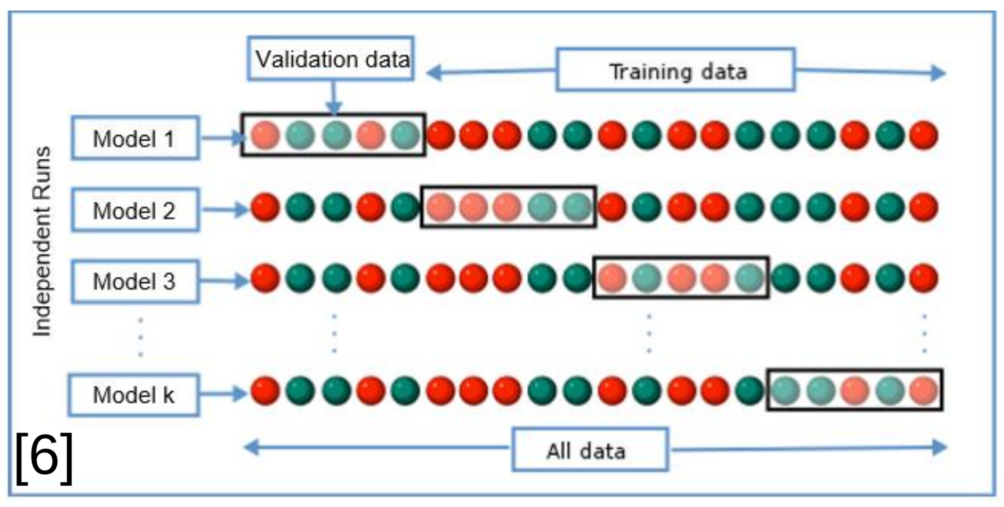
* Normalized by both indentation depth and load

Random Forest Regression (RFR)	Kernel Ridge Regression (KRR) [2]	Residual Multi Fidelity Neural Network (RMFNN) [3-4]
Description: Combination of an Assembly of weak learners (randomized decision trees)	**Description:** Regularized Linear Regression	**Description:** Combination of two Neural Networks merged by trainable parameters
Characteristics: Easy to implement (**scikit-learn**) Easy to interpret → Feature importance Only few hyperparameters Trees are build in parallel	**Characteristics:** Easy to implement (**scikit-learn**) Explicit solution	**Characteristics:** Can learn from multi fidelity data Transfer-Learning possible Implemented in (**DeepXDE**) Used Optimizer RADAM

Results and Discussion:

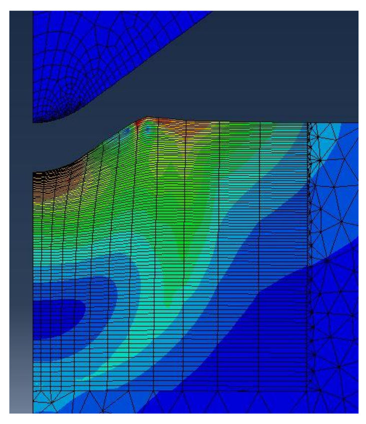
MAPE - Mean Absolute Percentage Error

$$MAPE = \frac{1}{N}\sum_{i=1}^{N}\left|\frac{y_{True} - y_{Predict}}{y_{True}}\right|$$

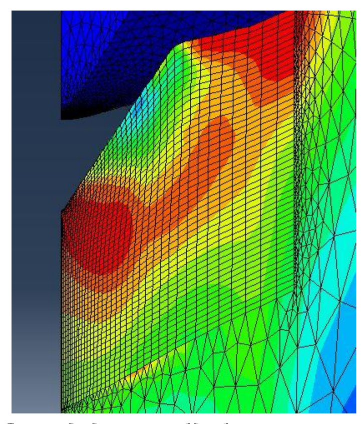


[6]

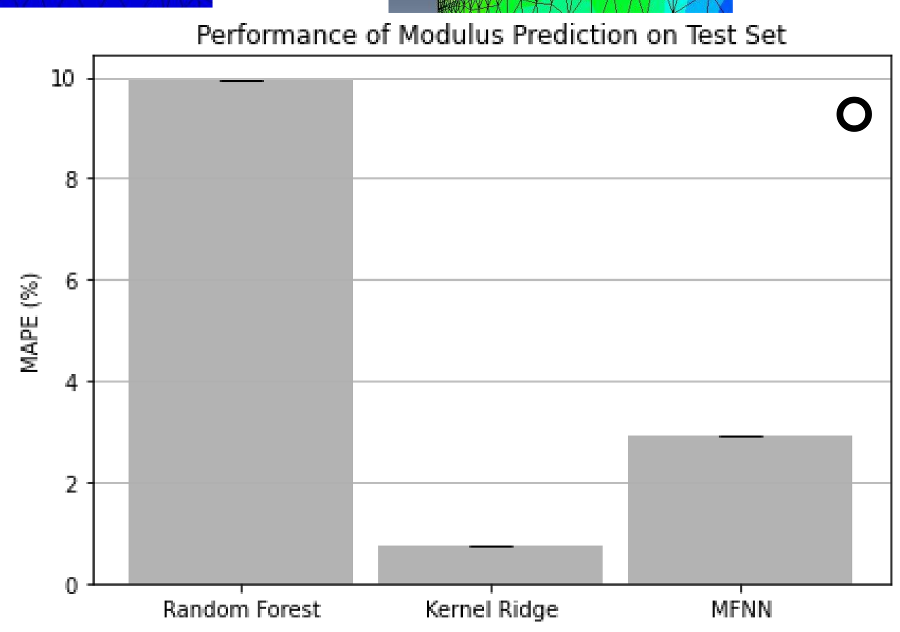
2D Simulations → Low fidelity

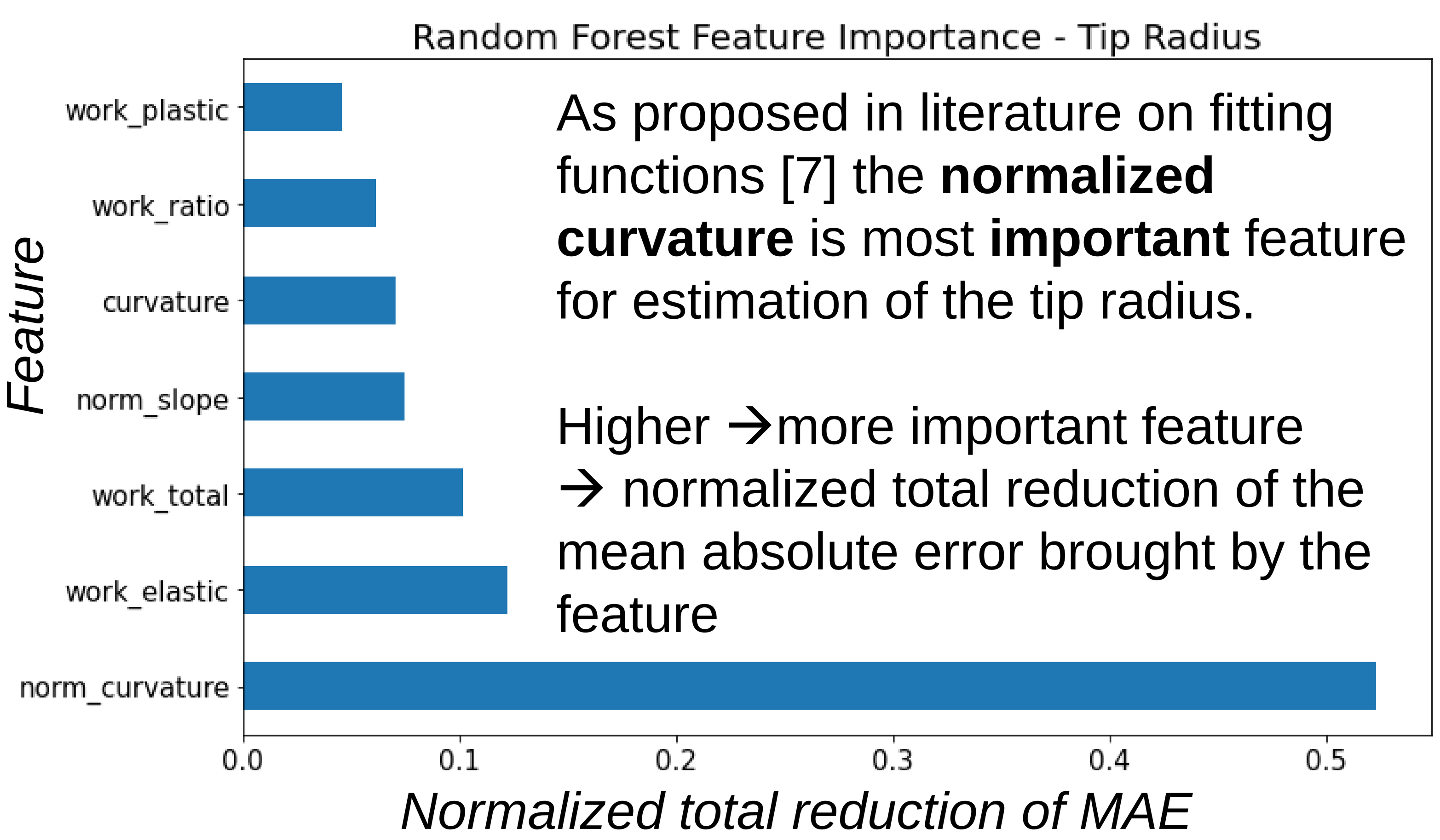


High fidelity 3D data



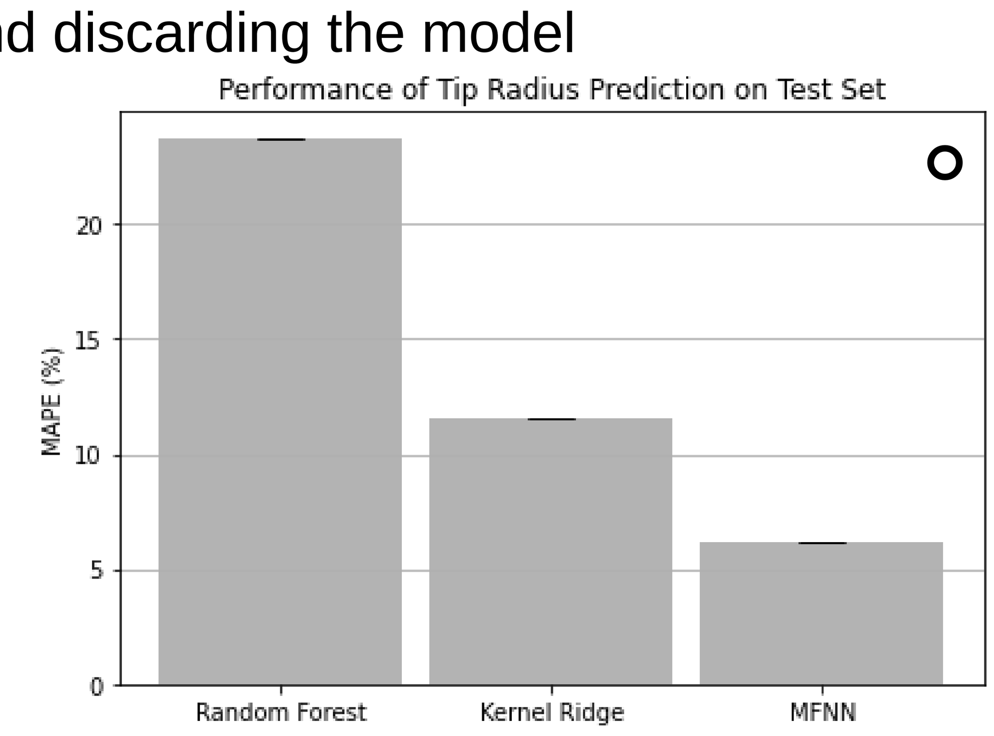
Grid Search Cross Validation used as implemented in scikit-learn to find best hyperparameters →performance estimation of ML models on a limited data sample → subsampling different trainings and validation sets → training and discarding the model



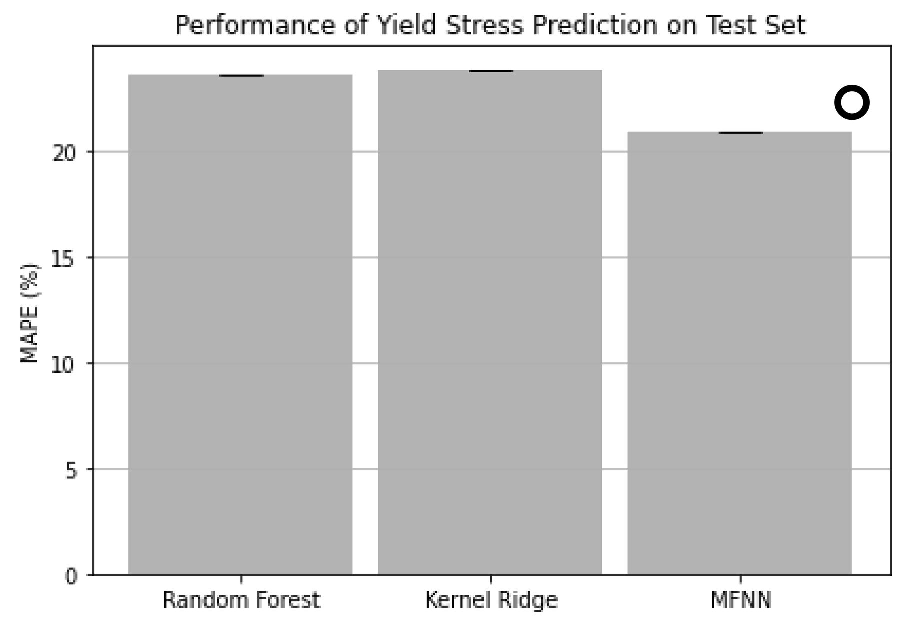


As proposed in literature on fitting functions [7] the **normalized curvature** is most **important** feature for estimation of the tip radius.

Higher →more important feature → normalized total reduction of the mean absolute error brought by the feature



○ RFR/KRR trained on best features for respective method. MFNN trained with a combination of important features for 2D & 3D obtained from best of KRR



Conclusion/Critique/Future Outlook

- General problem of indentation still apply. True mystical pairs (different elasto-plastic properties similar indentation curve) can be possible, they could lead to incorrect predictions [8,9]. Therefore, critical evaluation of the materials properties is still needed.
- We have shown that machine learning algorithms are able to learn from simulations data and predict materials properties with high accuracy, accounting for the tip-radius effects and also allowing tip-radius estimations.
- Applying the technique to experimental data will allow insights to tip wear during experiments, allowing just in time replacement of the tip.
- **High potential for interpretation of thin film data** is expected. We expect similar approaches to enable **correction for substrate influences.** Sub-micron films have less microstructural differences, e.g. sputtered films grow columnar and the fabrication method and size restrictions minimize the possibility of severe different local microstructures. Therefore, the local properties could potentially approximate the global properties.

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