A Pointwise Evaluation Metric to Visualize Errors in Machine Learning Surrogate Models

ML1381

Poster Presentation (MLIS 2021)

Seyed Shayan Sajjadinia[1]
ssajjadinia@unibz.it

Bruno Carpentieri[1]
bruno.carpentieri@unibz.it

Gerhard A. Holzapfel[2,3]
holzapfel@tugraz.at

[1] Faculty of Computer Science, Free University of Bozen-Bolzano, Bozen-Bolzano, 39100, Italy
[2] Institute of Biomechanics, Graz University of Technology, Stremayrgasse 16/2, Graz, 8010, Austria
[3] Department of Structural Engineering, Norwegian University of Science and Technology (NTNU), Trondheim, Norway

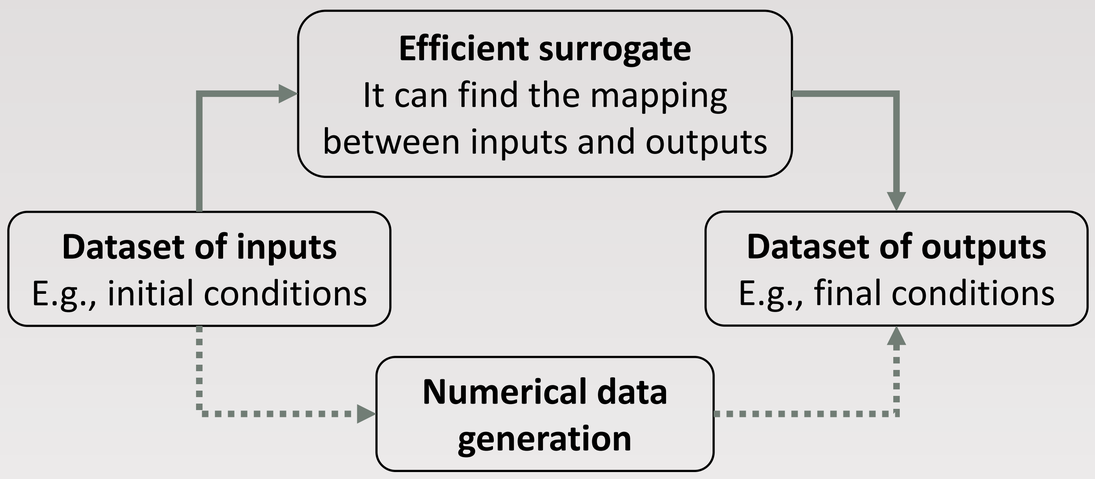
Introduction

We need numerical methods for physics-based simulation, but they can be repetitive and expensive [1-4]. Fortunately, simple and high-performance machine learning surrogates can replace them [4]. Nevertheless, with current metrics, e.g., the mean squared error (MSE), they can barely be interpretable, and for that reason, we propose the pointwise MSE (PMSE).

Methodology

The figure below shows a typical high-performance supervised surrogate that is trained by machine learning on a subset of previously generated numerical data. This can eventually be used instead of the expensive numerical model.

A typical supervised machine learning surrogate



The surrogate may be evaluated on the testing sets by the MSE or our PMSE metrics:

$$\mathbf{MSE} = \frac{1}{MN}\sum_{m=1}^{M}\sum_{n=1}^{N}\left(\bar{y}_{m,n} - y_{m,n}\right)^2$$

$$\mathbf{PMSE}_n = \frac{1}{M}\sum_{m=1}^{M}\left(\bar{y}_{m,n} - y_{m,n}\right)^2$$

M: number of test samples
N: number of material points
n: considered point
m: considered sample
$\bar{y}_{m,n}$: prediction
$y_{m,n}$: target

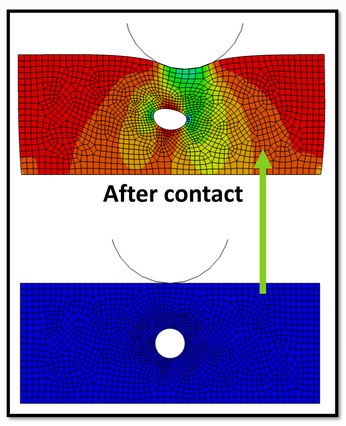
PMSE is pointwise; therefore, it is more interpretable than MSE.

PMSE is used only for testing; therefore, it is as efficient as MSE.

Experimental Setup

A feed-forward neural network is trained for surrogate modeling of a numerical contact problem (as shown on the right). The inputs are the material behavior and movements of the contacting indenter. The vertical stresses from the outputs roughly represent the loading effect in the vertical direction in the model.

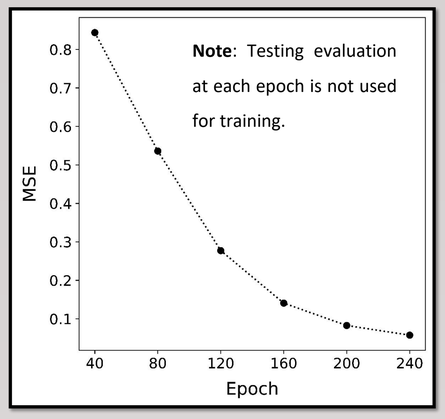
Numerical model of a contact problem



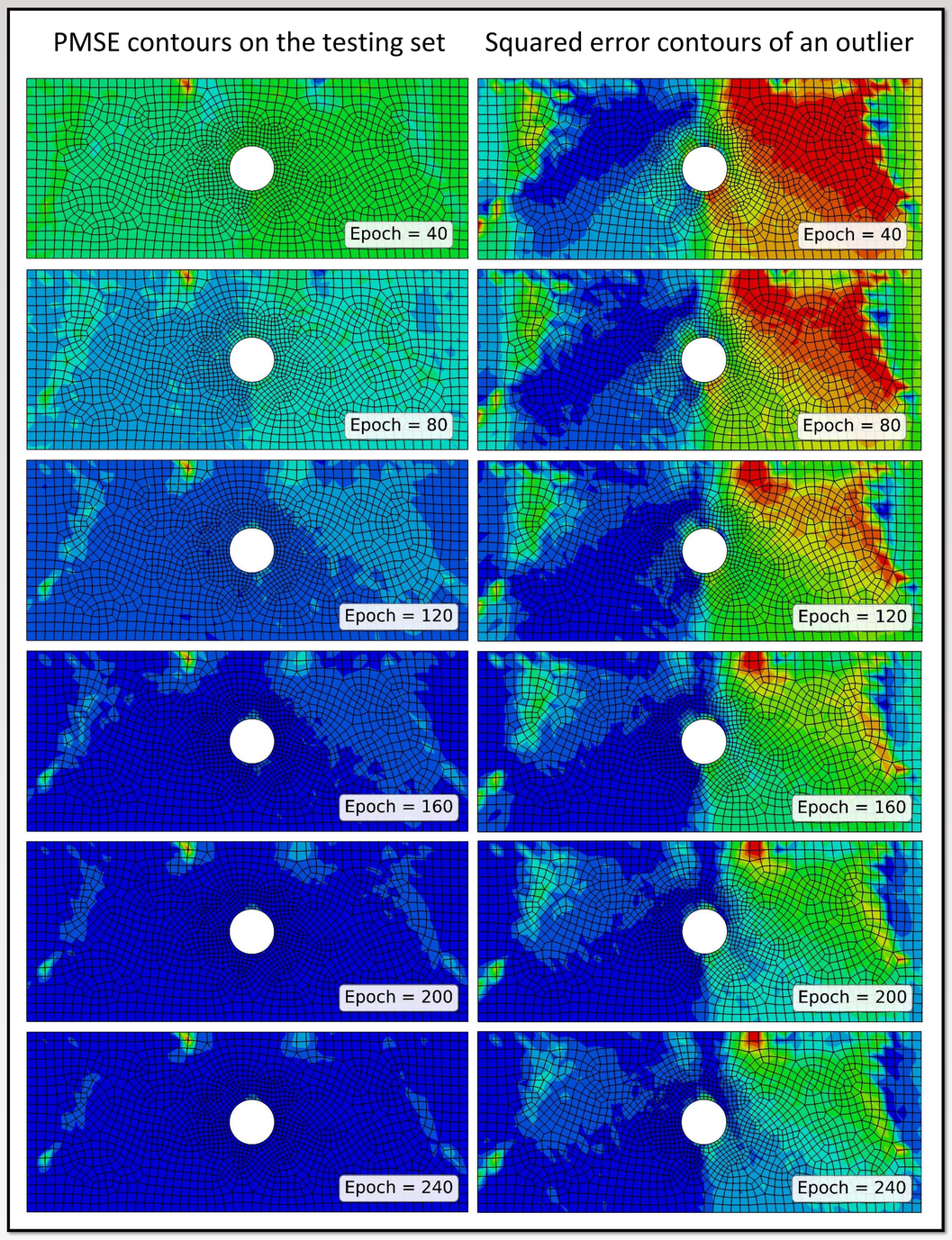
Results

The surrogate, enabling real-time simulation, was evaluated several times (after training), using the MSE (see the right figure). Below, we compare the PMSE with the error in one outlier, mapped onto the initial configuration.

MSE on the testing set



Comparison of two pointwise evaluation methods



Conclusions

- Our simple and efficient PMSE metric can present further complementary (and possibly generalizable) information about the machine learning performance.
- It may also reveal the correlation between numerical modeling and learning progress.

References

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