Physics-Enhanced Multi-fidelity Learning for Optical Surface Imprint

Yongchao Chen YONGCHAOCHEN@FAS.HARVARD.EDU
School of Engineering and Applied Sciences
Harvard University
Cambridge, MA 02138, USA

Abstract

Human fingerprints serve as one unique and powerful characteristic for each person, from which policemen can recognize the identity. Similar to humans, many natural bodies and intrinsic mechanical qualities can also be uniquely identified from surface characteristics. To measure the elasto-plastic properties of one material, one formally sharp indenter is pushed into the measured body under constant force and retracted, leaving a unique residual imprint of the minute size from several micrometers to nanometers. However, one great challenge is how to map the optical image of this residual imprint into the real wanted mechanical properties, i.e., the tensile force curve. In this paper, we propose a novel method to use multi-fidelity neural networks (MFNN) to solve this inverse problem. We first actively train the NN model via pure simulation data, and then bridge the sim-to-real gap via transfer learning. The most innovative part is that we use NN to dig out the unknown physics and also implant the known physics into the transfer learning framework, thus highly improving the model stability and decreasing the data requirement. This work serves as one great example of applying machine learning into the real experimental research, especially under the constraints of data limitation and fidelity variance.

Keywords: Active Learning, Sim-to-real Transfer, Inverse Problem

1. Introduction

Over the past century, humans have been searching for the optimal natural or artificial materials with most suitable mechanical properties. To accelerate this searching process, persistent research has focused on developing platforms for high-throughout (HT) synthesis and characterization of materials (Ament et al., 2021; Erps et al., 2021). Benefiting from its intrinsic experimental simplicity and broad applicability, indentation has been considered as a paradigm for HT probe of mechanical properties of materials (Chen et al., 2021; Lu et al., 2020). Using one sharp indenter to push into the material surface under the constant load, the material surface will be crashed to form a crown-like pattern which contains plentiful information to reveal elasto-plastic properties of materials. However, since the inverse mapping from the crashed pattern into formal material parameters is quite complex, many former researchers regard the pattern information as a rough criterion (Jeong et al., 2021). Herein, we attempt to optimize the inverse mapping from the residual pattern formed by indentation into the formal stress-strain curve of materials through MFNN. To make sure our problem is not ill-conditioned so that the model can predict well, we first apply NN to explore the forward problem and then combine the optimization method to search the possibility of non-uniqueness. This method assists to determine what suitable features to choose. Our scientific discovery is that instead of choosing the load-displacement curve, the residual pattern is already informative enough for predicting stress-strain relation.

Machine learning has many applications such as robotics (Chen et al., 2023b; Zhou et al., 2022), autonomous driving (Chen et al., 2023a; Zhou et al., 2023), and natural language processing (Chen et al., 2023c). As for the NN architecture, the whole process is achieved by first building up an initial NN model based on a large amount of 2D simulation data through finite element methods (FEM), and then transferring it into the 3D model using some 3D FEM simulation data. To mitigate the data requirement, the simulation data are augmented actively based on the prediction errors (Konyushkova et al., 2017). The transferred model gets further fine-tuned by incorporating some real experimental data and corresponding physical constraints into the model. To make the transfer learning process more efficient and stabilized, two physical parameters (friction coefficient μ and Poisson's ratio ν) are tuned in the simulation set, resulting into an ensemble of three parallel NNs. The final model is constructed from these NNs. It turns out that this step of tuning physical parameters is quite critical to the prediction accuracy. The underlying principle is owing to the closer sim-to-real gap after tuning the friction coefficient μ and Poisson's ratio ν. The final result owns satisfying accuracy when predicting the real stress-strain relation of the testing materials. In summary, the main contributions of the paper include:

- To the best of our knowledge, the first attempt to apply NN framework to inverting the optical profile of the indentation imprint to the real material elasto-plastic properties.
- Designing the MFNN framework to combine multi-fidelity data from 2D and 3D FEM simulation, and real experiments. Incorporating the physical intuitions into the MFNN model to decrease the data requirements and stabilize the model.
- Applying forward NN and BFGS (Yuan, 1991) optimization to explore the non-unique issue in the inverse problem and dig out the required features for training.

2. Backgrounds and methods

Figure 1 schematically illustrates the problem set of our study. Figure 1A (left side) is a schematic diagram showing a typical stress-strain response of a power-law strain-hardening material which can be used for many engineering metallic materials. The elastic behavior follows Hook's law, whereas the plastic response is approximated by different constitutive models (Hertelé et al., 2011). One assumption is the three-parameter Hollomon model (fitting parameters: E, σ_y, n), in which true stress σ and true strain ε are related as:

$$\sigma = \begin{cases} E\varepsilon, & \sigma < \sigma_y \\ E\varepsilon_y^{1-n}\varepsilon^n, & \sigma \geq \sigma_y \end{cases} \tag{1}$$

, while another assuming model is the four-parameter Ludwik model (fitting parameters: E, σ_y, n, K), displayed as:

$$\sigma = \begin{cases} E\varepsilon, & \sigma < \sigma_y \\ K\varepsilon_p^n, & \sigma \geq \sigma_y \end{cases} \tag{2}$$

, where E is the elastic modulus, σ_y is the yield stress, K is the work hardening coefficient, n is the work hardening exponent, and ε_p is the equivalent plastic strain determined as $\varepsilon_p = \varepsilon - \dfrac{\sigma}{E}$.

Knowing the stress-strain relation of one material, theoretically we can uniquely determine the residual imprint and load-depth curve. This is referred as the forward problem. However, how to inversely determine the stress-strain curve from the residual imprint remains challenging.

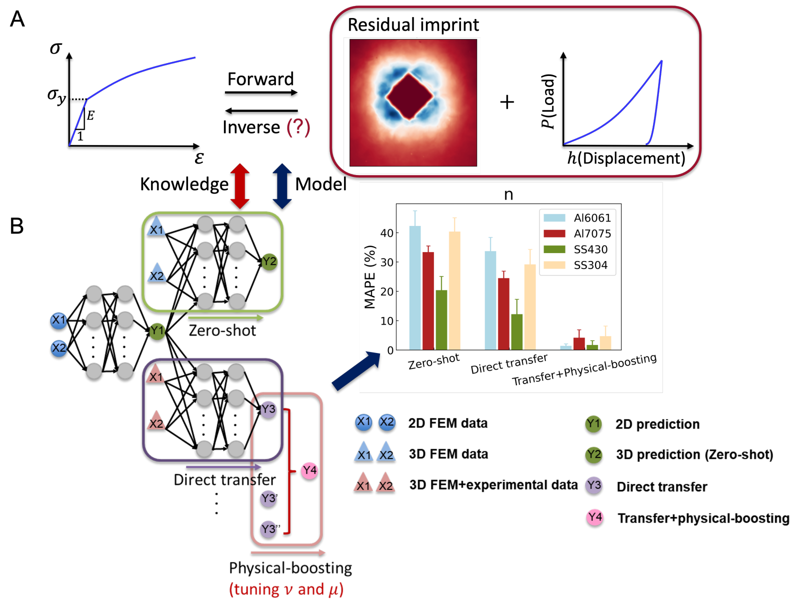

Figure 1: Transfer learning to solve the indentation inverse problem via residual imprint (pile-up). (A) Schematic illustration of indentation forward and inverse problems. Materials conforming to typical hardening behaviors (left) will form pile-up on sample surfaces after indentation and response typical load-displacement curves (right). (B) Flowcharts of the transfer learning DNN employed in this study.

3. Experiments and results

3.1 Unique problem and feature selection

One fundamental question is whether the features we choose can guarantee a unique problem. Here we artificially define the feature extraction method based on curve characteristics. Specifically, we can extract three features from force curves based on the the loading curvature, initial unloading slope, and the ratio of residual unloading depth to maximum loading depth. We extract nine features from pile-up curves by finding the maximum height and calculating the volumes and weighted centres in varied parts. We also have tried using encoder-decoder structure to automatically output features, while the testing results show that both types of features perform similarly.

As shown in Figure 2E, we use 2D FEM data to build up an accurate forward prediction model, i.e., predicting the force and pile-up features based on input constitutive model parameters. The data number is actively augmented to ensure that the Mean Absolute Percentage Error ($MAPE$) for predicting each feature is below 2%. Each time 50 data points are added into the parameter range with large errors, and the total data number for forward prediction is 2450. Then we use this trained NN as a surrogate model to explore the informativeness of the indented features. To check whether one material owns siblings with quite similar features, we fix its parameters and iterate the parameters of the candidate material to continually decrease their feature differences. The iteration process uses typical BFGS optimization algorithm. The iteration stops when the $MAPE$ of all features are below the set limit or the iteration number exceeds the upper limit. Finally, we carry

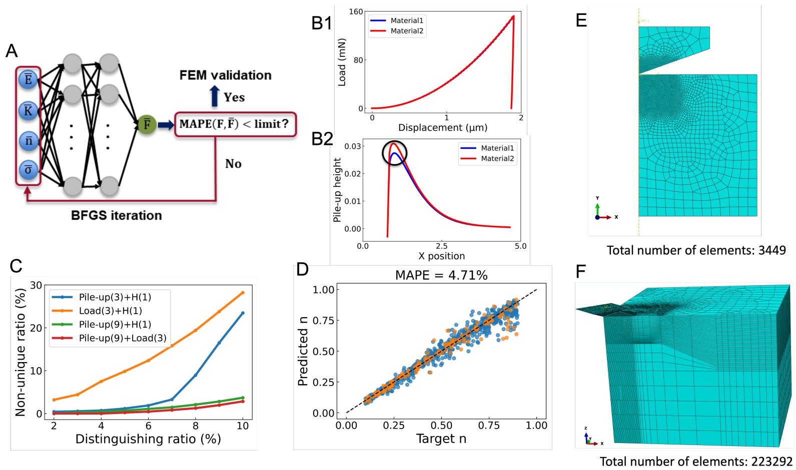

Figure 2: Forward prediction with the unique problem and inverse prediction with the feature selection process.

out FEM simulations to verify whether the hypothesized material siblings own similar features. Figure 2B1 and Figure 2B2 display two typical material siblings acquired from the above-mentioned workflow, in which the load-displacement curves are almost the same and the pile-ups reveal some difference at the highest parts.

Theoretically, we can distinguish two materials if the maximum difference among their features exceeds the possible variance, e.g., the experimental errors. Hence, we define the concept of distinguishing ratio as,

$$Distinguishing\ ratio = \max_{i=1,2,\ldots,N} \left| \frac{F_i - \bar{F}_i}{F_i} \right| \tag{3}$$

, where F_i and $\bar{F}_i$ are the features from two material siblings, respectively. N depends on how many features considered. We then take a uniform grid (grid number = 5) on the parameter space of Ludiwk model, and test the uniqueness of 625 materials. Among these 625 materials, N_A of them own material siblings with all the relative feature differences lower than the distinguishing ratio. Then we define the non-unique ratio at this specific distinguishing ratio as $N_A/625$, displaying the possibility to encounter unique problems. Figure 2C shows the evolution of the non-unique ratio with the distinguishing ratio employing different features. It reveals that the unique problem is quite severe if only three force features and hardness are input as features. However, the non-uniqueness is largely mitigated if we also include the information of pile-up. Even if we choose only three features from pile-up combined with hardness, the performance is still much better than the pure force case when the distinguishing ratio is lower than 6%. Meanwhile, we find that the non-unique ratios with nine pile-up features and three force features are close to the case with nine pile-up features and hardness, both observing slight increases when the distinguishing ratio is higher than 8%. This hints that when including the information of pile-up, maybe we can represent the information of load-displacement relation with only hardness. We then verify this hypothesis by doing the inverse training with nine pile-up features and hardness. The $MAPE$ of each predicted parameter (E, σ_y,

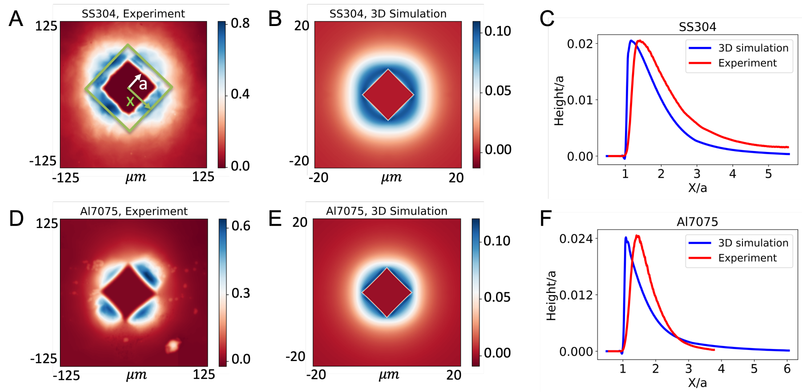

Figure 3: Pile-up profiles acquired from experiments and simulations. (A-C) and (D-F) are pile-up profiles of SS304, and Al7075, respectively.

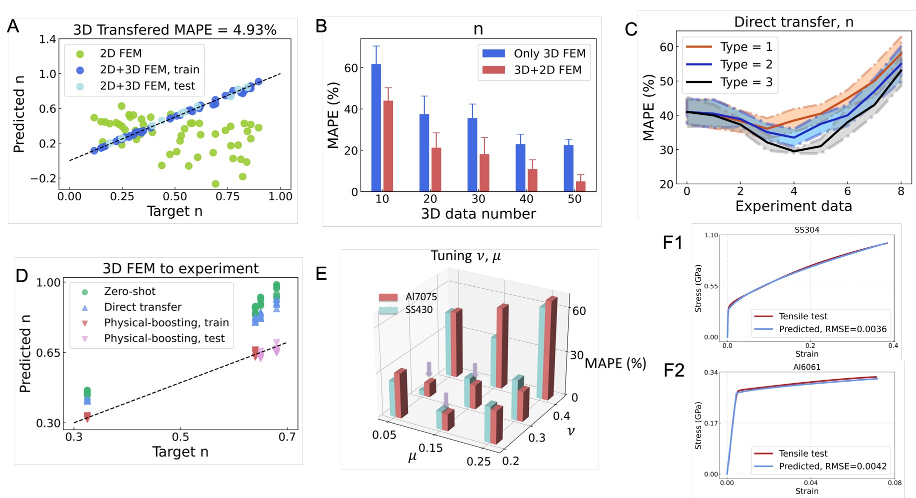

Figure 4: A transfer learning framework for the real experimental prediction.

n, K) for the testing set decreases to lower than 5% when the total data number increases to 4000, as shown in Figure 2D.

3.2 2D to 3D simulation model transfer

Figure 3A and Figure 3B show two typical 2D images of pile-up morphologies in the experiment and 3D FEM simulation, respectively. To mitigate the height variations and transform the 2D image into the 1D curve, we divide the 2D image into many slim square strips and calculate the average height in each divided region. Then we acquire a plot of the averaged height vs. the distance to the imprint center and calculate related features, as shown in Figure 3C.

Since different shaped indenters will result to different pile-up morphologies and corresponding features, using the ML model trained by the 2D FEM data to predict the 3D FEM result will contain large errors. We first use 4000 2D FEM data to build up a 2D ML model and directly employ it for the prediction of 3D FEM results, denoted as $Y1$ in Figure 1. The green points in Fig. 4A display the prediction of n in this case, and the errors are quite large. However, these predicted Y1 still incorporate the information of 2D FEM data, and they own a rough trend with the true values. To correct the wrong correspondence and transfer the model from 2D to 3D, here we set the predicted $Y1$ as the extra feature and put it together with the original pile-up features and hardness extracted from 3D FEM model to predict the target parameters (E, σ_y, n, K). Figure 4B shows the evolution of MAPE vs. the 3D data number for the case with and without the extra feature ($Y1$). We find the MAPE of the case incorporating 2D prediction will decrease to lower than 5% when the data number increases to 50, much lower than the case using pure 3D data. Figure 4A shows the correspondence of the predicted and targeted values based on this transferred model. The transfer learning framework decreases the requirement of expensive data.

3.3 Sim-to-real model transfer (Physical-boosting)

We plot the evolution of MAPE with the experiment data number in Figure 4C. Among total 4 types of materials, the number of materials used for the training ranges from 1 to 3, respectively. With the experiment data number increasing, the MAPE will first decrease and then increase when the experiment data number exceeds 4, implying overfitting. According to the above discussion, the transfer learning will be inefficient if the experimental data is rare and the sim-to-real gap is too large. In the above FEM simulations, the Poisson's ratio ν and the friction coefficient μ are always assumed to be fixed values (ν = 0.3, μ = 0.15), which are common settings in most indentation models (Chen et al., 2007; Goto et al., 2019; Haj-Ali et al., 2008). We vary the ν to be (0.2, 0.3, 0.4) and the μ to be (0.05, 0.15, 0.25), and then calculate the evolution of pile-ups in these 3^2 cases. Figure 4E displays the total feature differences between simulations and experiments under varied ν and μ. Among the nine combinations, the sim-to-real gap will be lower than others if the two physical parameters (ν, μ) = [(0.3, 0.15), (0.3, 0.05), (0.2, 0.15)]. Next, we build up three independent DNNs in which the input 3D FEM data are calculated by setting two physical parameters to be the above three values, respectively.

Then for each DNN, using the merged data of 3D FEM and experiments, one candidate value will be predicted, denoted as $Y3$, $Y3'$, $Y3''$ in three independent subsets. These three DNNs form into a committee and finally determine what the optimal prediction value is. The specific weights for each DNN are tuned as,

$$Y4 = \alpha 1 * Y1 + \alpha 2 * Y2 + (1 - \alpha 1 - \alpha 2) * Y3 \tag{4}$$

Here $Y4$ is the final predicted value in our model and ($\alpha 1$, $\alpha 2$) are two parameters to be determined by experimental data. We use this final model to predict the stress-strain relation in the left two materials SS304 (Figure 4F1) and Al6061 (Figure 4F2), serving as the testing set. The predicted stress-strain curves are satisfyingly close to the real curves acquired by tensile testing.

4. Discussion

Herein, we attempt to bridge the gap between optical residual profiles and material elasto-plastic properties via MFNN. How to use machine learning to explore the inverse problem and how to supplement the physical constraints into the model are discussed. Active learning and transfer learning are used to mitigate the sim-to-real gap with least data.

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