Prediction of Composite Microstructure Stress Distribution Using a Machine Learning Approach

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Abstract

The objective of this study is to predict stress distribution in composite materials using machine learning approach. Finite Element Analysis is the widely used method for structure and material behavior analysis. However, this method is computationally expensive when applied to composite materials or when non-linear features are involved. Thus, Machine Learning (ML) techniques can offer a good and efficient alternative for complex problems. Compared to previous works, the method used in this study is a differential-base neural network method which means that instead of predicting the stress contour, the neural network framework predicts a stress difference using reference stress contour then the actual stress distribution is reconstructed. The obtained results show the efficiency of neural network in the prediction of the stress distribution in complex structures. The calculated prediction error was equal to 25% and 22% at the level of the fibers and the matrix, respectively. This study also provides a parametric study on the impact of the size of the validation set and the density of the cartesian map on the prediction error.

1 Generation of data

In order to get the datasets, we had two options. The first option consists of creating our own microstructures and run Finite Element Simulations using ABAQUS to get the stress distribution. The second option was to use datasets from published studies.

We started with a literature review on previous works on the application of Machine Learning for the prediction of mechanical properties of composites. Very few studies examined the application of machine learning for stress prediction and most of them are very recent [1,2,3,4]. Thus, we used the study of Feng et al. [3], one of the most recent studies, as a reference. The two-phase composite consists of fiber reinforced polymer composite. We assume that the matrix has a linear elastic behavior with Young's modulus and Poisson's ration equal to 3.2 GPa and 0.3 respectively, which correspond to epoxy resin. Similarly, we assume that carbon fibers have a linear elastic behavior with Young's modulus and Poisson's ratio are equal to 8 GPa and 0.35 respectively. We restrain the horizontal displacement and the vertical displacement on the bottom-edge and the left-edge of the model. A compressive displacement of 0.1 μm is applied on the top-edge. Finite Element simulation are performed to get the stress distribution in the composite.

2 Processing of data

In this study, we are interested in the prediction of von Mises stress contour. Once we get the stress distribution from finite element analysis, one of the observations was that the stress contour and the microstructural geometry don't have the same size (see Fig.1). In fact, due to the variation of the fibers' locations, each microstructural model deformed in a different way under the applied displacement. That is why we need to interpolate the stress contour onto a Cartesian Map, as proposed by Feng et al. [3], so that all contours have the same size that is the initial model size of 10 μm by 10 μm. Several methods can be used to interpolate the contour onto the Cartesian Map. In this work, Barycentric coordinate system-based interpolation method was used. Each node on the Cartesian map was projected on the Finite Element mesh, then the triangle in which the node falls was determined and then the stress corresponding to that node was calculated using the stresses at the three vertices of the triangle. The following equations are used to determine the Barycentric parameters λ_1, λ_2, λ_3 and the stress at the Cartesian Map node S [3]:

$$\lambda_1 = \frac{(y_2 - y_3)(x - x_3) + (x_3 - x_2)(y - y_3)}{(y_2 - y_3)(x_1 - x_3) + (x_3 - x_2)(y_1 - y_3)}$$

$$\lambda_2 = \frac{(y_3 - y_1)(x - x_3) + (x_1 - x_2)(y - y_3)}{(y_2 - y_3)(x_1 - x_3) + (x_3 - x_2)(y_1 - y_3)}$$

$$\lambda_3 = 1 - \lambda_1 - \lambda_2$$

$$S = \lambda_1 S_1 + \lambda_2 S_2 + \lambda_3 S_3$$

Where x_i, y_i, $i = 1, 2, 3$, and x, y are the coordinates of the triangle vertex and the Cartesian Map node coordinates, respectively. S is the interpolated stress at the Cartesian Map node and S_1, S_2, S_3 are the stresses at the nodes of the triangular mesh element.

The steps of the generation and the processing of data are presented on figure 1. We illustrate an example of the training geometry and stress distribution that we obtained using ABAQUS. Figure 1 also shows the interpolated stress contour. The interpolated stress contour is then stored in a file where for each Cartesian map node we have the associated stress and the associated property P, such that

$$P = \begin{cases} 1 & \text{if the Cartesian Map node lies on the matrix} \\ 2 & \text{if the Cartesian Map node lies on the fiber} \end{cases}$$

Since the generation and the processing of data is time consuming, we are going to use the training data provided in the study conducted by Feng et al. [3]. The dataset used in this study consists of 1000 distinct microstructures. the microstructures have the same number of fibers and the same material parameters. The location of the fibers is the only parameter that varies.

80 % of the dataset was used for the training set, 10% for the validation set and 10% for testing.

3 Neural network framework

The Neural Network framework that we used in this study consists of three main parts: first the stress processing module, followed by the Encoder-Decoder module which is the main core of the code and the last part is the stress prediction. Compared to other existing frameworks, the method used in this work is based on the definition of a reference stress state and the prediction of the stress difference, since this approach has been shown to provide better accuracy [3,5]. The blocks of the Neural Network framework can be described as follows:

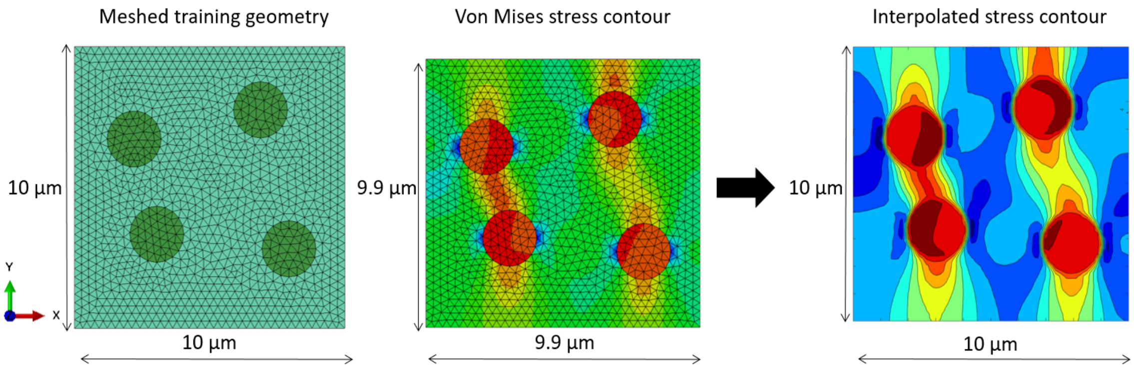

Figure 1: (a) The geometry (b) The stress distribution under 0.1 microns compressive displacement (c) The interpolated stress contour

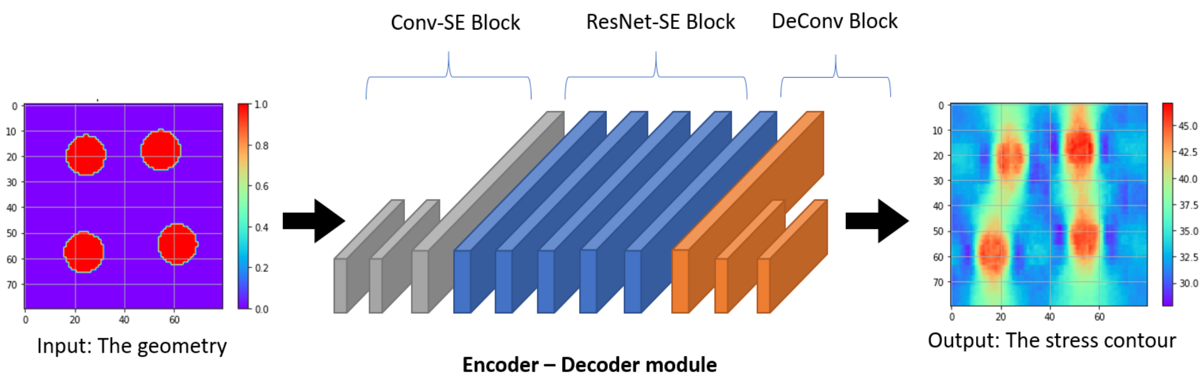

Figure 2: The blocks of the neural network framework

- **Data processing**: the objective of this module is to calculate the stress difference. A reference stress state is selected and is kept fixed throughout the study. the data processing block determine the difference between a given stress contour and the reference stress contour. The Encoder-Decoder module uses the stress difference as input instead of the original stress contour.
- **Encoder-Decoder**: it consists of three blocks illustrated in figure 2: Conv-SE (SE = Squeeze-and-Excitation block), ResNet-SE and DeConv. The objective of this section is to first extract high level features from the processed data, then model the inter-dependencies. ResNet-SE block will then improve the extracted dependent high level features. Finally, the deconvolutional layers will reconstruct the initial input dimension using the key features.
- **Stress prediction**: Once the Encoder-Decoder predicts the stress difference, the objective of this block is to generate the predicted stress contour using the stress reference.

In order to measure the prediction error, we decided to rely on the maximum nodal stress. The errors were calculated separately for the fibers and the matrix. The average prediction error was calculated as follows

$$MaximumStressError = MSE = \frac{1}{N}\sum_{i=1}^{N}\frac{|max(S_i) - max(\bar{S}_i)|}{max(\bar{S}_i)} \tag{1}$$

Where S_i is the predicted nodal stress and $\bar{S}_i$ is the nodal stress given by FEA.

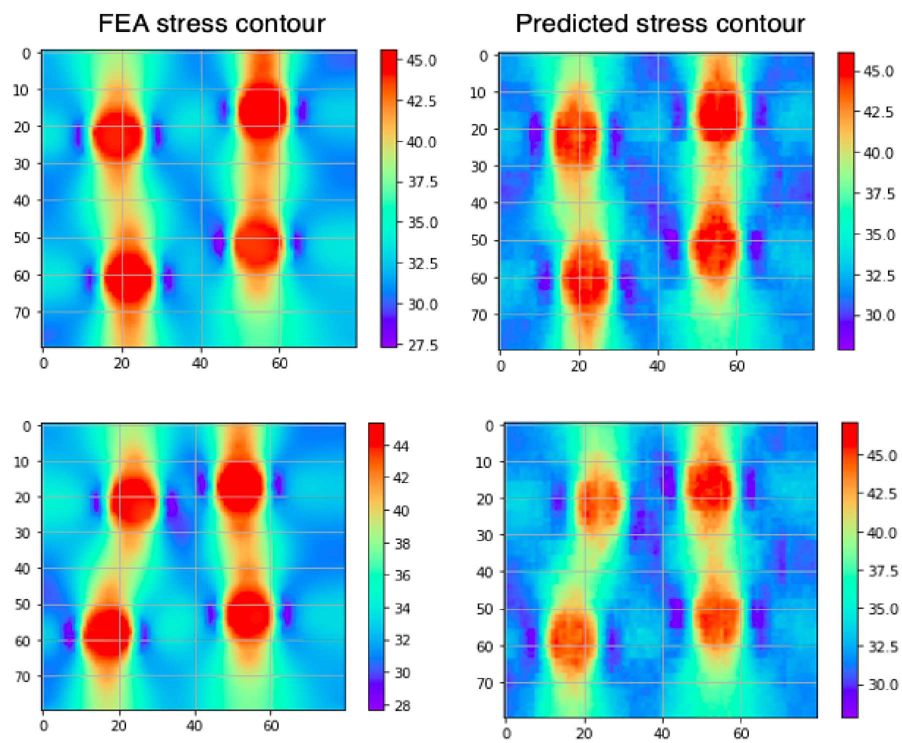

Figure 3: Comparison of the stress contour obtained from FEA and Neural Network framework

4 Results

4.1 The predicted stress contour

Figure 3 compares the stress contours obtained using finite element analysis and the stress contour obtained using neural network approach. We can see that the stress prediction obtained using neural network is in good agreement with finite element analysis. The obtained test prediction error is equal to 25% and 22% at the level of the fibers and the matrix, respectively.

Figure 4 shows the convergence of the testing and training loss as we increase the number of Epoch which is a good indicator to track cases of over-fitting and under-fitting. Both test and training loss converged after 7 Epochs which indicates that the model is well-fitted.

We also compared the prediction during of Neural Network framework to the duration required by FEA software ABAQUS to run the analysis on one sample. Neural Network framework takes 1.5 sec to predict the stress contour for one sample whereas FEA needs 7 sec. Thus, neural network framework managed to considerably decline the analysis duration.

4.2 Parametric study

Additionally, we conducted a parametric study on the impact of the size of the validation set and the density of the Cartesian Map on the test prediction error. Figure 5 illustrates the evolution of the test error measured for the fibers and the matrix as we decrease the size of the validation set. We can conclude that the adequate ratio for the validation set is equal to 10%. Figure 6 presents the variation of the test error and the training duration as a function of the density of the Cartesian Map. The results show that there is an optimum at which the lower error is achieved, that is for a Cartesian Map of 80-by-80. Figure 6 also shows that the training duration increases as we increase the density of the Cartesian Map, which is completely predictable. The training duration moved from 33 minutes for a 64-by-64 CM to 92 minutes for 120-by-120 CM.

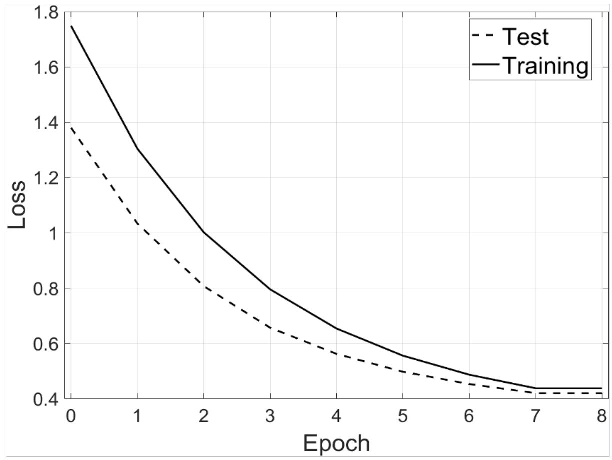

Figure 4: Training and test loss as a function of the number of Epochs

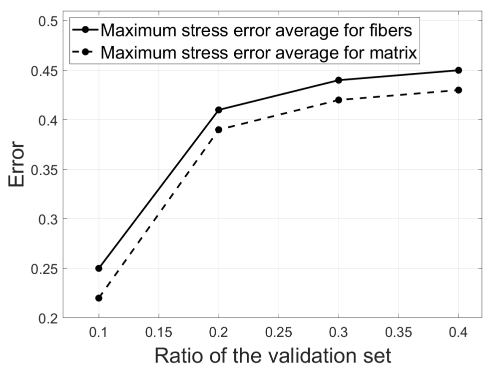

Figure 5: Impact of the validation set size on the test error

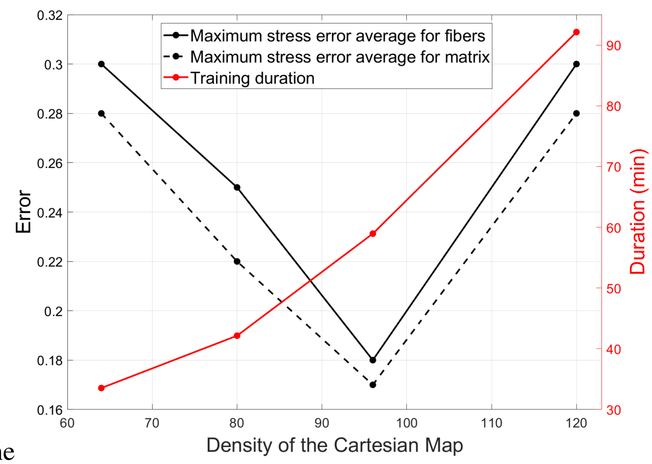

Figure 6: The impact of the density of the Cartesian Map on the test error and training duration

5 Conclusions

This study shows that Neural Network framework based on stress difference is able to accurately predict the stress distribution in composite materials. The conclusions of this work can be summarized as follows:

- The prediction error is equal to 25% and 22% for the fibers and the matrix, respectively.
- The prediction duration for one sample is equal to 1.5 sec, while for FEA it takes 7 sec to get the stress distribution for one sample. Thus, Neural Network framework managed to significantly decrease the analysis duration.
- The lowest prediction error is obtained using a validation set ratio of 10%.
- The training duration is highly affected by the density of the Cartesian Map.
- There is an optimum size for the Cartesian Map (i.e. 80-by-80) at which the lowest prediction error is achieved.

This framework can furthermore be applied on composites with highly random fiber distribution to test its efficiency and propose any potential required improvements.

6 Contributions

Marwa Yacouti: This project was conducted individually.

References

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