Predicting FRP Mechanical Properties through CNN-based Microstructure Analysis

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Final Presentation

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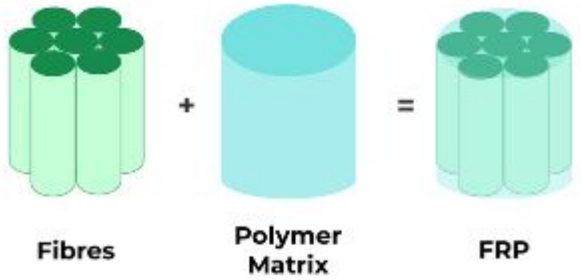
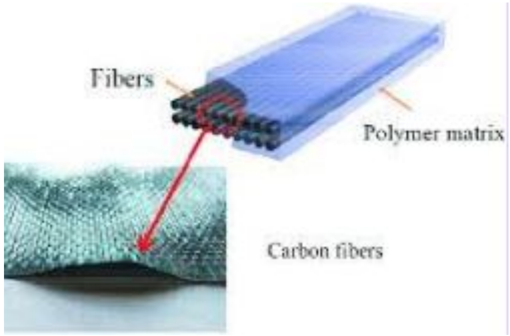
Problem Statement

- Fiber-reinforced polymers (**FRP**) are widely used due to their high strength and lightweight properties.
- **Predicting** mechanical properties of FRP based on microstructure is challenging due to complex interactions between fibers and matrix.
- This research paper proposes a **CNN-based** approach to extract features from microstructure images of FRPs and predict their mechanical properties.
- The **aim** is to provide an **accurate** and efficient method for **predicting** the mechanical properties of FRP materials that can help in design and optimization of these materials for various applications.

FRP = Fibre Reinforced Polymer

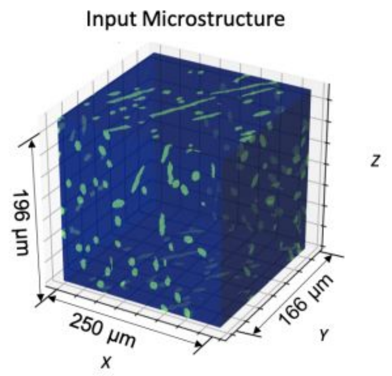
- composite material
- consists of **polymer matrix**, such as epoxy or polyester
- **reinforced** with **fibers**
- fibers used - carbon, glass, aramid, or basalt, etc.
- these fibers provide **strength** and **stiffness** to the composite material

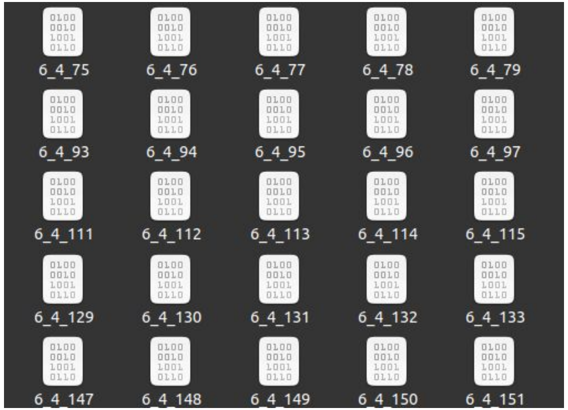


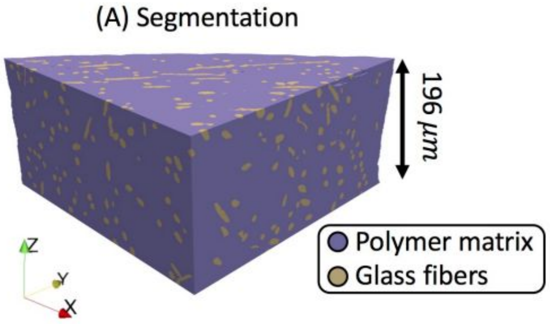


Data Set and Microstructure Images

- **5321 2D** microstructure slices and its corresponding z-normal stress distribution
- each slice is stored in a numpy array with the filename being the corresponding coordinates values
- sampled from **segmented X-ray tomography** images of a composite specimen
- exact microstructure of a fiber-reinforced thermoplastic composite was analyzed
- Injection-molded composite
  - polymer matrix - polypropylene
  - fiber fillers - E-glass fibers





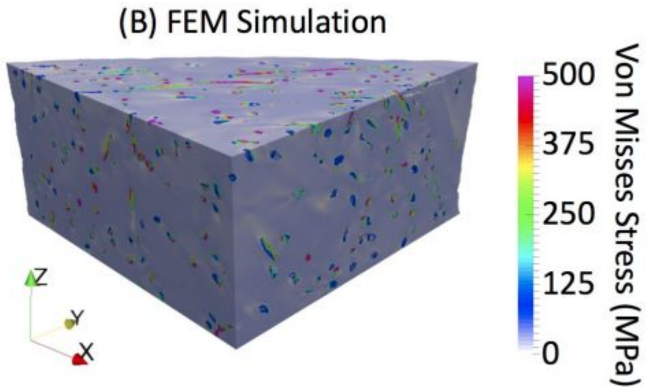


- The E-glass fibers
  - diameter 10 μm
  - had varying lengths and orientations in the final composite specimen
- The injection molded part
  - cylindrical rod with a diameter of 1.27 cm and a length of 45.72 cm
- the injection molding direction was in the length direction of the cylinder
- the cylindrical rod was then machined into a smaller dog-bone shaped specimen with a gauge section diameter of 2.5 mm, and a gauge section length of 5 mm.

About the FES existing in research

- Focused on four features
  - the exterior edge of the specimen,
  - the glass fibers,
  - the porosity, and
  - the polymer matrix

- 92.5 hours!!



Deep Learning Framework

1. Data Sampling
2. Preprocessing
3. Network Architecture
4. Network Training
5. Evaluation Metrics

Data Sampling

- segmented microstructure represented by **unit-less square voxels** and a tetrahedral mesh element FE simulation.
- **Stress field data** was resized to match the segmented data using the **scipy.ndimage.zoom** method via order **3 spline interpolation**.
- Data points were selected from the segmented microstructure and corresponding stress field, with a sampling window size of **32x32 pixels** to contain the entire fiber's cross-section and serve downsampling purposes.
- Each data point was stored in a **rank 3** array of shape **(32, 32, 2)**, with the third axis representing the voxel microstructure type and stress value.
- three different planes (xy-plane, xz-plane, and yz-plane) to investigate the importance of sampling plane to the model performance.

Preprocessing

- Sampled data points randomly split into:
  - Training set = 80%
  - Testing set = 20%
- Standardised the model input using:
  - $X\_norm = X - \mu\_train \,/\, \sigma\_train$
- Sample mean and standard deviation with the same shape as the input in the training set

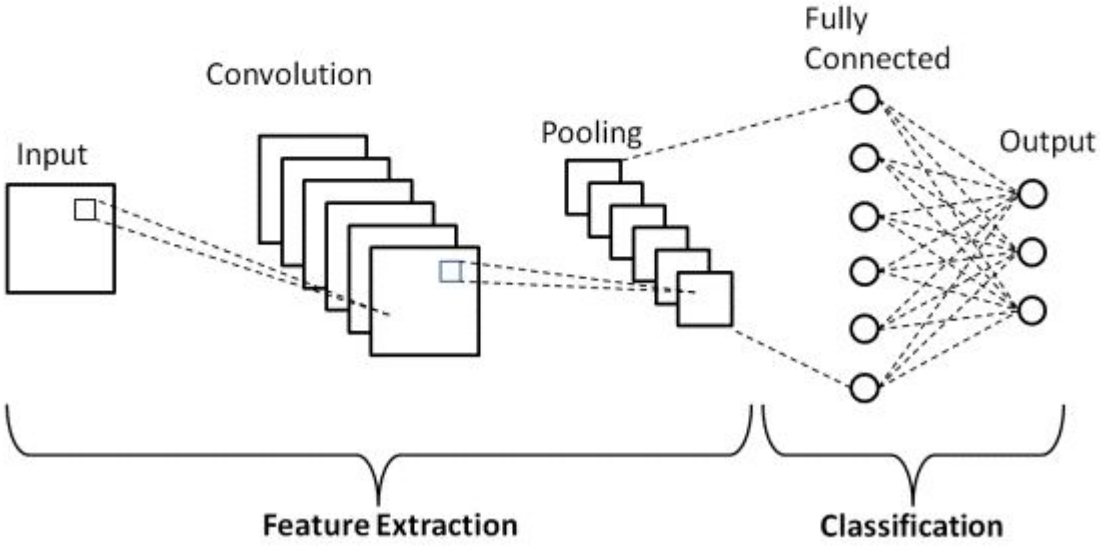
Description of ML methodology, CNN

- commonly used for image classification and **object recognition tasks**

- consist of multiple layers of filters that learn features from the input images

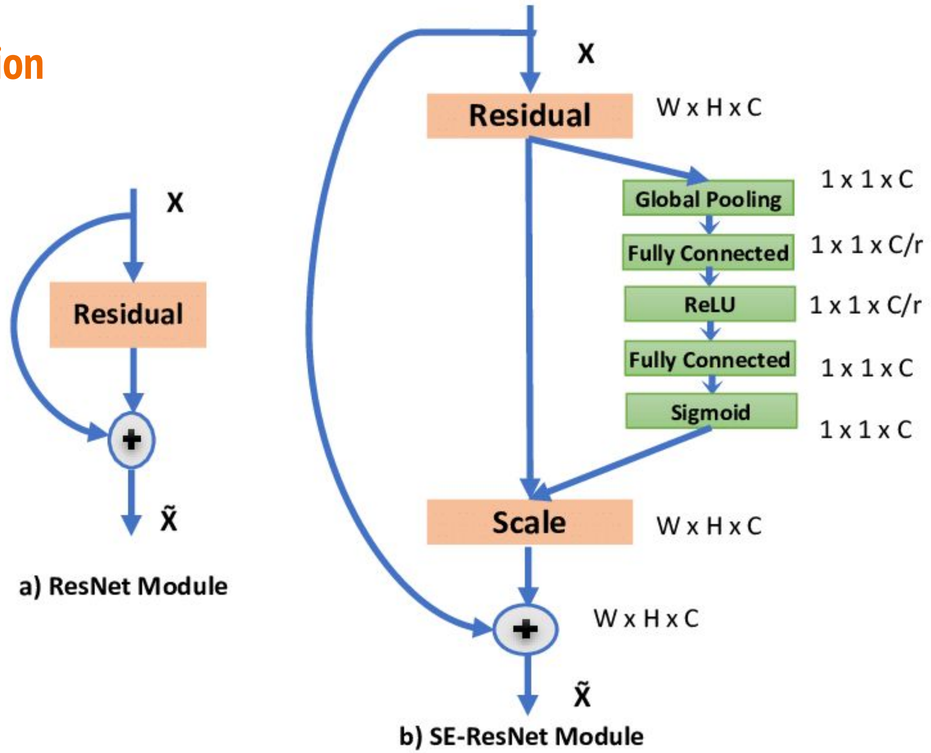
- learned features are then used to classify the images into different categories or predict numerical values, such as mechanical properties

- but, the paper has modified this and we are using a novel CNN method -> **SE ResNet**



SE ResNet

Squeeze and Excitation



Network Architecture

- **StressNet** - used for stress field identification in linear elastic materials

- In the study, StressNet is adopted and **modified** to extend to the **non-linear mechanical** behavior of fiber-reinforced polymers.

- The network
  - an input layer
  - an output layer
  - 11 hidden layers in between

- The input was the segmented microstructure array of size $\mathbf{32 \times 32}$, denoted by X

- Feature maps by : $\boldsymbol{Si = Wi \star X + bi}$

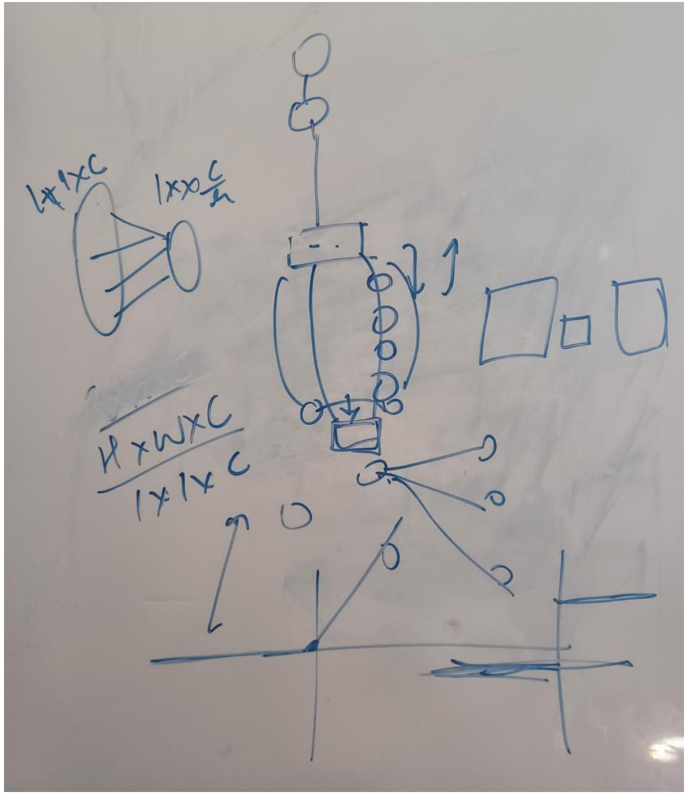
Network Training (contd.)

- At the end of each convolutional layer, an activation function was applied on the feature maps = ReLU

- The formulation of the ReLU was $\boldsymbol{ReLU(s) = \{\, s, \text{ if } s > 0}$
  $\boldsymbol{0, \text{ Otherwise}}$
  where s was the entry of the feature map matrix Si

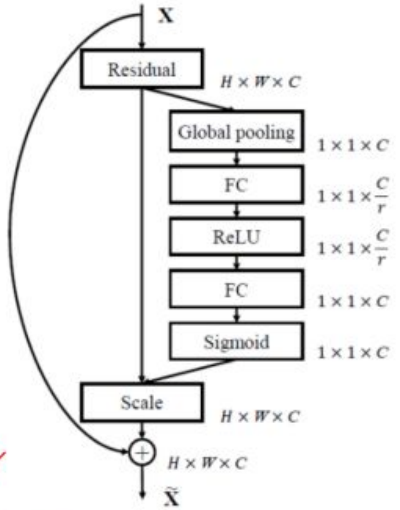
- $\boldsymbol{dReLU\ /\ ds = \{\, 1, \text{ if } s > 0}$
  $\boldsymbol{0, \text{ Otherwise}}$

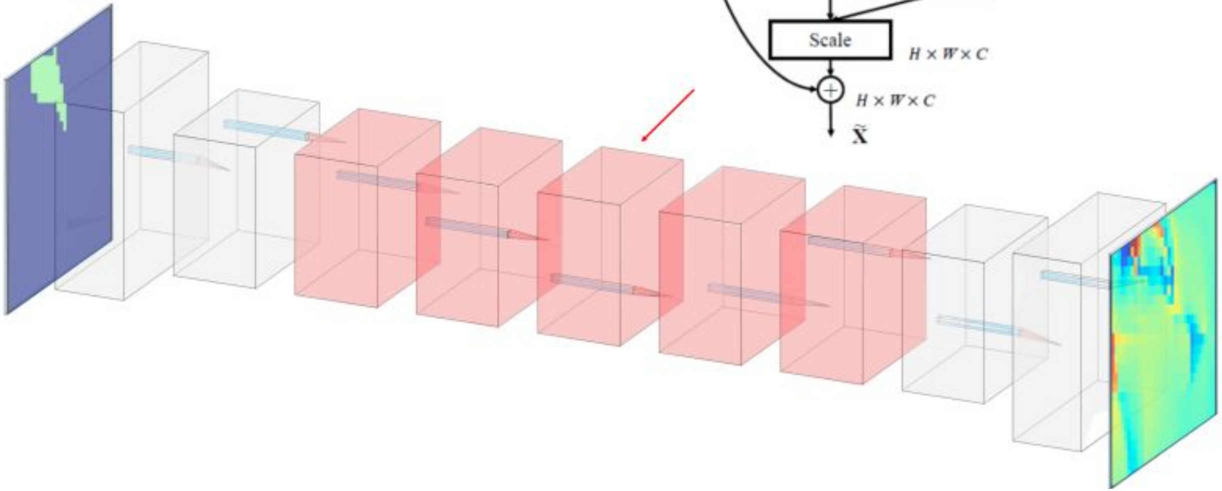
- The final output of each convolutional layer
  - $O = ReLU(Si\,) = ReLU(Wi \star X + bi\,)$



Operation Layers		Number of Filters	Kernel Size	Stride	Padding	Output Size
Input Segmented Microstructure		-	-	-	-	$32 \times 32 \times 1$
Convolution Layer	ReLU	32	3×3	1×1	SAME	$32 \times 32 \times 32$
Pooling	Max pooling	-	2×2	2×2	SAME	$16 \times 16 \times 16$
Convolution Layer	ReLU	64	3×3	1×1	SAME	$16 \times 16 \times 64$
Pooling	Max pooling	-	2×2	2×2	SAME	$8 \times 8 \times 64$
SE ResNet Layer	ReLU	64	3×3	1×1	SAME	$8 \times 8 \times 64$
SE ResNet Layer	ReLU	64	3×3	1×1	SAME	$8 \times 8 \times 64$
SE ResNet Layer	ReLU	64	3×3	1×1	SAME	$8 \times 8 \times 64$
SE ResNet Layer	ReLU	64	3×3	1×1	SAME	$8 \times 8 \times 64$
SE ResNet Layer	ReLU	64	3×3	1×1	SAME	$8 \times 8 \times 64$
Transposed Convolution	ReLU	64	3×3	2×2	SAME	$16 \times 16 \times 64$
Transposed Convolution	ReLU	32	3×3	2×2	SAME	$32 \times 32 \times 32$
Convolution Layer	-	1	3×3	1×1	SAME	$32 \times 32 \times 1$
Output Stress Field		-	-	-	-	$32 \times 32 \times 1$

Table : Network Architecture





CNN architecture with an encoder-decoder structure. This network takes microstructure images of size 32 × 32 as input and outputs the corresponding stress field of the same size. The red highlighted blocks are Squeeze-Excitation Residual blocks and the rest are plain 2D convolution layers with MaxPooling.

Evaluation Matrix

- coefficient of determination
  - $R2 = 1 - SSres/SStot$
    - $SSres = \sum (f - y)^2$
    - $SStot = \sum (y - \bar{y})^2$

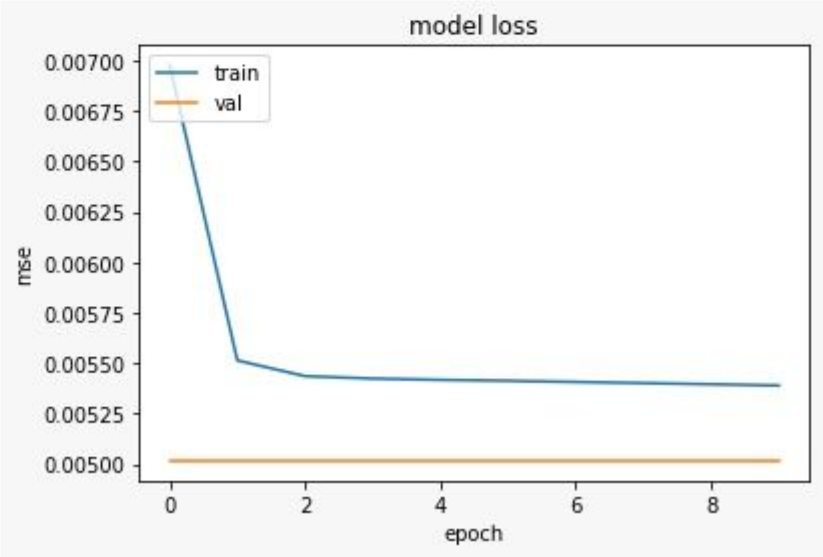
- $f =$ predicted values from the CNN model

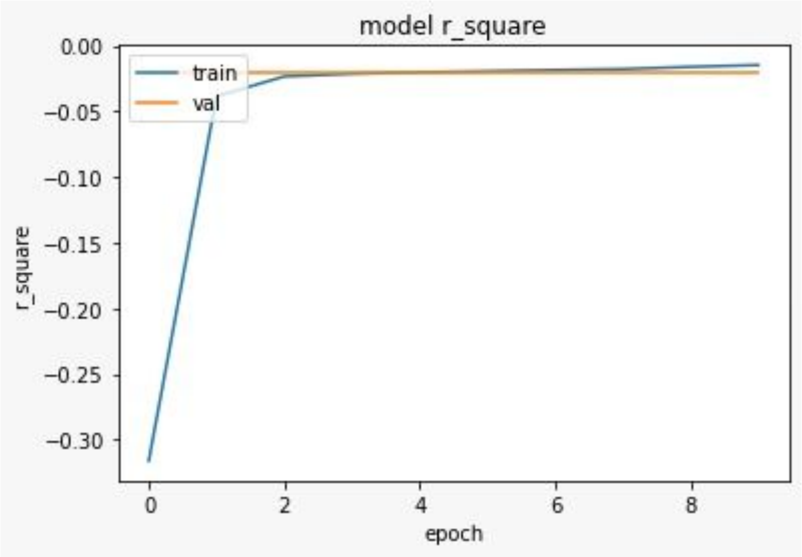
- $y =$ true values in the FE dataset

- $\bar{y} =$ sample mean of y

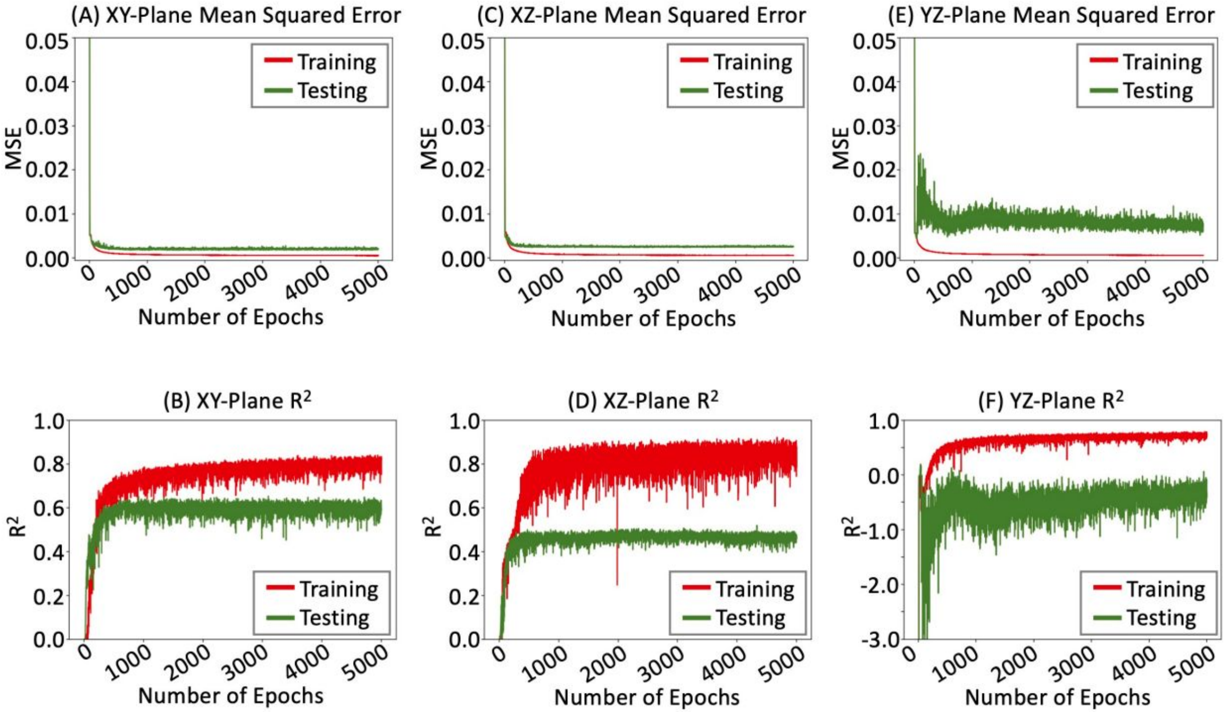
- perfect model is expected to have an $R2$ of 1

Our results!


model loss
train
val
mse
0.00700
0.00675
0.00650
0.00625
0.00600
0.00575
0.00550
0.00525
0.00500
0
2
4
6
8
epoch


model r_square
train
val
r_square
0.00
−0.05
−0.10
−0.15
−0.20
−0.25
−0.30
0
2
4
6
8
epoch

Exploring paper's results



Interpretation of current results

Model training on 2D slices sampled from the xy-plane resulted in **decreasing MSE values** for both training and testing sets as epochs increased.

After around **400** epochs, the MSE values stabilized with a slightly higher testing error than training error.

Conversely, the training process measured in R2 showed increasing scores on both training and testing sets as the number of epochs increased.

The curves for R2 scores also became flat after approximately 400 epochs, indicating a higher R2 score for the training set compared to the testing set.

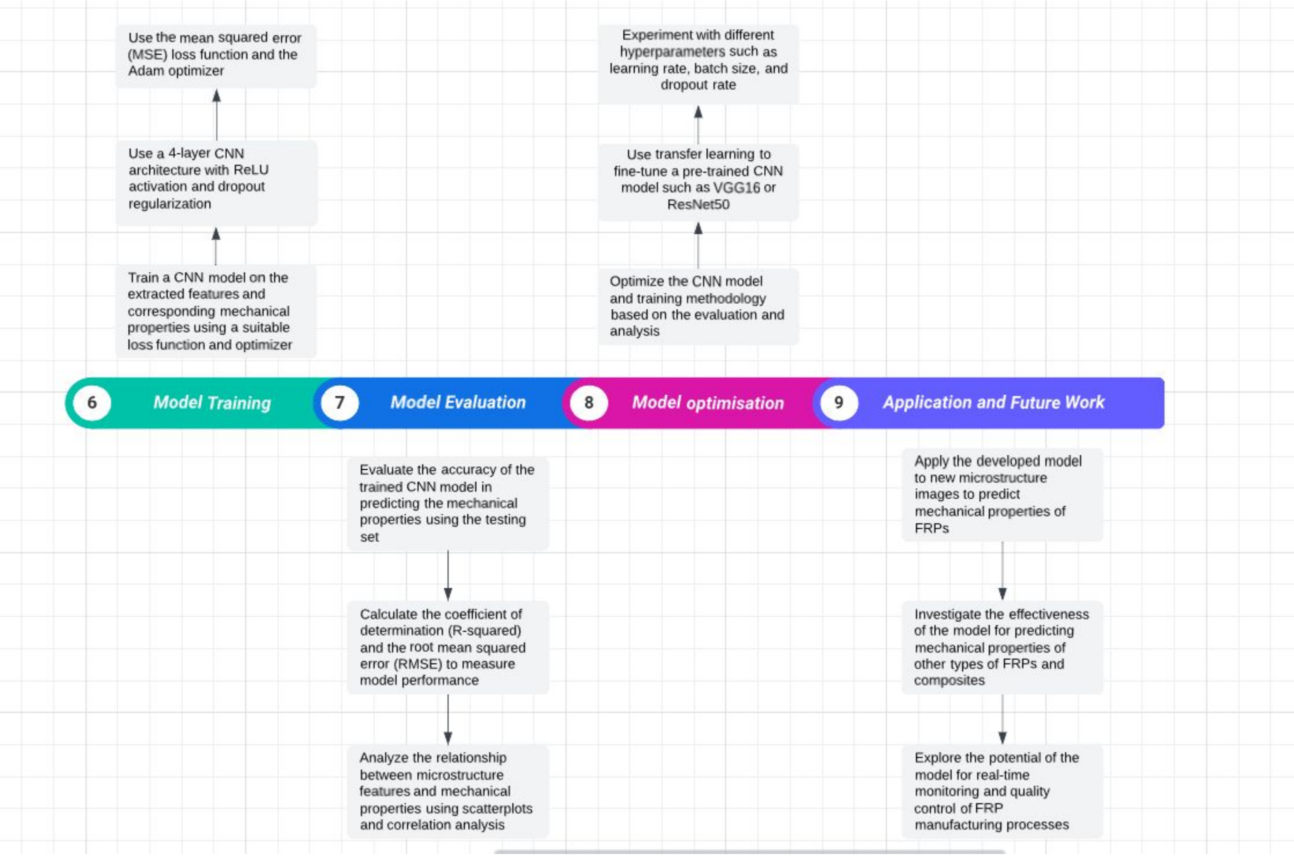
In summary, the model exhibited stable MSE values with a slightly higher testing error than training error, while the R2 scores showed increasing trends with higher scores for the training set compared to the testing set.

Conclusion

- The study aims to create a model that uses segmented microstructure as input and generates σzz as output.
- The same network architecture was used to train models on data points sampled from different planes (xy, yz, and xz).
- The datasets from the three planes were of the same size and contained 5321 data points each.
- The models were trained with 5000 epochs using batch-normalization.
- The training process showed that MSE values decreased as the number of epochs increased, and the curves became stable after around 400 epochs.
- The $R2$ scores increased with the number of epochs, and the curves became flat after around 400 epochs, corresponding to a higher $R2$ score for the training set compared to the testing set.

References

1. Predicting Mechanical Properties from Microstructure Images in Fiber-reinforced Polymers using Convolutional Neural Networks Yixuan Suna , Imad Hanhanb , Michael D. Sangidb and Guang Linc,∗ [link]


Use the mean squared error (MSE) loss function and the Adam optimizer
Use a 4-layer CNN architecture with ReLU activation and dropout regularization
Train a CNN model on the extracted features and corresponding mechanical properties using a suitable loss function and optimizer
Experiment with different hyperparameters such as learning rate, batch size, and dropout rate
Use transfer learning to fine-tune a pre-trained CNN model such as VGG16 or ResNet50
Optimize the CNN model and training methodology based on the evaluation and analysis
6
Model Training
7
Model Evaluation
8
Model optimisation
9
Application and Future Work
Evaluate the accuracy of the trained CNN model in predicting the mechanical properties using the testing set
Calculate the coefficient of determination (R-squared) and the root mean squared error (RMSE) to measure model performance
Analyze the relationship between microstructure features and mechanical properties using scatterplots and correlation analysis
Apply the developed model to new microstructure images to predict mechanical properties of FRPs
Investigate the effectiveness of the model for predicting mechanical properties of other types of FRPs and composites
Explore the potential of the model for real-time monitoring and quality control of FRP manufacturing processes