USING DEEP LEARNING TECHNIQUES TO PREDICT EFFECTIVE DIFUSIVITY OF POROUS MEDIA FROM IMAGES

Thesis submitted in partial fulfilment

of

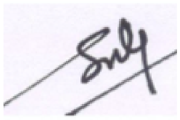
Masters in Technology

in

Chemical Engineering

By

SAURABH KUMAR PANDEY



(17CH30055)

Under the guidance of

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November - 2021

DECLARATION

I certify that the work contained in this report entitled "**USING DEEP LEARNING TECHNIQUES TO PREDICT EFFECTIVE DIFUSIVITY OF POROUS MEDIA FROM IMAGES**" is original and has been done by me under the guidance of my supervisor, Prof. Somenath Ganguly. The work has not been submitted for any purpose to any other university or institute. Whenever I have used materials (i.e. data, theoretical analysis, figures, and text) from other sources, I have given due credit to them by citing them in the text of the report and giving their details in the references.

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CERTIFICATE

This is to certify that the thesis entitled "**USING DEEP LEARNING TECHNIQUES TO PREDICT EFFECTIVE DIFUSIVITY OF POROUS MEDIA FROM IMAGES**", has been submitted to the Indian Institute of Technology, Kharagpur, in partial fulfilment of Master of Technology in Chemical Engineering Department at the Indian Institute of Technology, Kharagpur.

It is a faithful record of the work carried out by **Mr. Saurabh Kumar Pandey** (Roll no. **17CH30055**) under my supervision and guidance. It is further certified that no part of this report has been submitted to any other University or Institute for the award of any other Degree or Diploma.

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Date: 22/11/2021 Saurabh Kumar Pandey

Place: Kharagpur, India

CONTENTS

1. ABSTRACT

The application of machine learning is getting into the roots of every domain and this work reports the application of machine learning methods to predict effective diffusivity of porous media from their structure images. Convolutional Neural Networks have gained wide importance for image-based methods and we have tried to leverage the power of CNNs to develop a simple 2-layer neural network. The model built is optimized using hyperparameter tuning of different components of CNN like kernel size, number of filters, padding, activation functions, learning rate, etc. The optimized model has a relative error of ~30% on the validation set and ~39% on the test set. Further improvements in the score include more advanced methods such as introducing a physical factor like Porosity into the neural network and pre-processing the structure images to remove dead-end or trapped spaces to let the filters learn the features more suitably.

Keywords: Porous media, Effective Diffusivity, Convolutional Neural Network, Machine Learning, Hyperparameter tuning

2. INTRODUCTION

This work underlines the application of machine learning methods for predicting the effective diffusivity (*De*) of two-dimensional porous media from images of their structures [1]. The datasets generated from (lattice Boltzmann) LBM simulations are used to train convolutional neural network (CNN) models and evaluate their performance.

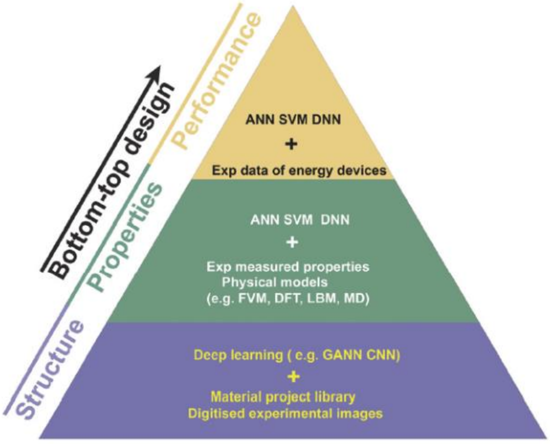

Fig.1 - AI-enabled structure reconstruction and generation, prediction of properties and in-service performance for porous energy materials

The effective transport properties of porous media are often computed using empirical correlations or effective medium theories with their structure information [2] (e.g., porosity) as input. Such an approach needs little computational cost and can be very accurate for some specific (often idealized) classes of porous media. It remains a great challenge to develop methods for predicting the effective transport properties of porous media that require low computational cost but offer high accuracy for diverse porous structures.

Machine learning can potentially be an effective approach for tackling the above challenge. Deep neural networks have demonstrated good predictive power when their input and output have important correlation with each other. Furthermore, image-based learning has been shown to be able to extract important physical features from images [3]. Because the effective transport properties (in particular, the effective diffusivity) of porous media is largely determined by their structure which can be conveniently represented using their binary images, conceivably, one can develop a surrogate deep learning model to extract key geometrical features from images of porous media and predict their transport properties. The prime objective of the work is stated as follows:

- Study of machine learning based approach to study different properties of porous media.
- Optimization of hyperparameters of a convolutional neural network to predict effective diffusivity of porous media.
- Improving the performance of neural networks through pre-processing pore structures or inducing physical properties like Porosity in the network

3. MODEL DEVELOPMENT

3.1. Dataset

Generated dataset is in CSV format as shown below. The file contains 301 binary images each with 16384 pixels (128*128) with pixel values of 0 and 1

	0	1	2	3	4	5	6	7	8	9	...	291	292	293	294	295	296	297	298	299	300
0	0	1	1	0	1	0	1	1	1	0	...	1	1	1	0	0	1	0	1	0	0
1	0	1	1	0	1	0	1	1	1	0	...	1	1	1	0	0	1	0	1	0	0
2	0	1	1	0	1	0	1	1	1	0	...	1	0	1	0	0	1	0	1	0	0
3	0	1	1	0	1	0	1	1	1	0	...	1	0	1	0	0	0	0	1	0	0
4	0	1	1	0	1	0	0	0	1	0	...	1	0	1	0	0	0	0	1	0	0
...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...
16379	0	1	0	0	0	0	0	0	1	1	...	0	0	0	1	1	0	0	0	1	0
16380	0	1	0	0	0	0	0	0	1	1	...	0	0	0	1	1	0	0	0	1	0
16381	0	1	0	0	0	0	0	0	1	1	...	0	0	0	1	1	0	0	0	1	0
16382	0	1	0	0	0	0	0	0	1	1	...	0	0	0	1	1	0	0	0	1	0
16383	0	1	0	0	0	0	0	0	1	1	...	0	0	0	1	1	0	0	0	1	0

16384 rows × 301 columns

The above dataset is converted into 128*128 binary images using OpenCV library in Python. Some sample images are shown below.

Fig. 2 - Sample dataset images. White color denotes pore space and black color denotes solid phase

The diffusivity values in the dataset can be described as follows. These values are normalized by a factor (1.958e-12) to get effective diffusivity for the porous media.

Mean	7.607423e-14
Std	3.261657e-14
Min	7.837232e-15
Max	2.948378e-13

Table. 1 – Description of Effective Diffusivity data

3.2. Data Pre-processing

Normalization – Since the diffusivity values are small, they are normalized by a factor (1.958 x 10^-12) to get all the values in the range 0-1

Train/Val/Test split – The data is split into train (80%), validation (10%) and test (10%). Training data is used to train images, validation data is used to select the model with best set of hyperparameters and test set is used to evaluate the model on test data.

3.3. Convolutional Neural Network Development

Of the many deep neural network models, convolutional neural network (CNN) is commonly applied to analyse visual imagery and has achieved much success in image classification. Recently, CNN has also been adopted to study the effective properties of complex materials and showed much potential for efficient and accurate prediction of a material’s effective properties from its structure. Prediction of permeability from images of porous media using CNN has provided useful insights in understanding the correlation between geometric features and transport properties.

A simple 2-layer CNN model is developed to study the images and derive physical insights from structures and these insights are used to develop a model that can be used to predict effective diffusivity of any given unknown porous media.

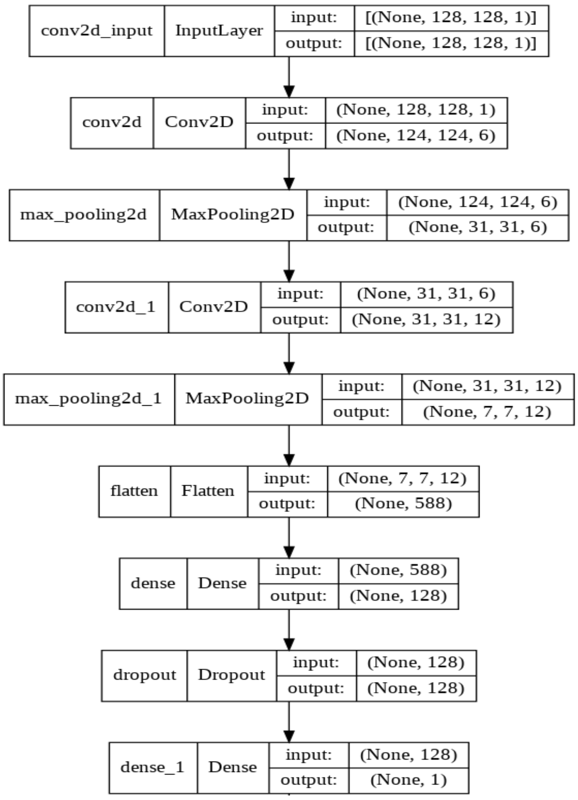

Fig. 3 - A simple 2-layer CNN model architecture.

Dense layer represents the Fully Connected layers and dense_1 is the final output to regress the model

Some CNN Terminologies

1. **Sequential model** – this model is used for a plain stack of layers where each layer has exactly one input tensor and one output tensor
2. **Convolution layers -** This layer creates a convolution kernel that is convolved with the layer input to produce a tensor of outputs.
3. **Max Pooling layers -** Downsamples the input along its spatial dimensions (height and width) by taking the maximum value over an input window for each channel of the input.
4. **ReLU Activation function** – Applies rectified linear unit activation : max(x, 0) on the input tensor.
5. **Padding -** one of "valid" or "same" . "valid" means no padding. "same" results in padding with zeros evenly to the left/right or up/down of the input such that output has the same height/width dimension as the input.
6. **Filters -** the dimensionality of the output space (i.e. the number of output filters in the convolution).
7. **Kernel size -** An integer specifying the height and width of the 2D convolution window.
8. **Dropout -** The Dropout layer randomly sets input units to 0 during training time, which helps prevent overfitting.
9. **Dense layers -** Dense layer is the Fully connected layer which implements the dot and multiplication operations on weight, input and bias matrices.
10. **Loss function -** Loss function used to regress the CNN model is Mean Squared Error (MSE), where y and y' are target and predicted values respectively.

$$\text{MSE} = \frac{1}{n}\sum_{i=1}^{n}(y_i - \tilde{y}_i)^2$$

11. **Performance Metric –** Relative error is used to measure and compare performance of different models.

$$\text{RE} = \frac{\text{Predicted value} - \text{Target value}}{\text{Target value}}$$

3.4. Hyperparameter Optimization

Kernel size	(2,2)	(3,3)	(4,4)	(5,5)
Learning Rate	1e-2	1e-3	1e-4	
Number of filters	(8,16)	(16,32)	(32,64)	
Strides	(2,2)	(3,3)	(4,4)	
Pool size	(2,2)	(3,3)	(4,4)	
Padding	"same"	"valid"		
Activation	ReLU	Linear		

Table 2 – Hyperparameters to be tested with CNN model

a. Linear Activation function

Kernel size	(4,4)
Learning Rate	1e-2
Number of filters	(8,16)
Strides	(3,3)
Pool size	(3,3)
Padding	"valid"
Activation	Linear

Table 3 – Hyperparameter configuration for best model with Linear Activation function

Train Set	35.79
Validation Set	30.73
Test Set	39.71

Table 4 – Train, Val and Test Relative Error for CNN with Linear Activation function

b. ReLU activation function

Kernel size	(5,5)
Learning Rate	1e-2
Number of filters	(32,64)
Strides	(3,3)
Pool size	(2,2)
Padding	"valid"
Activation	ReLU

Table 5 – Hyperparameter configuration for best model with ReLU Activation function

Train Set	39.66
Validation Set	36.39
Test Set	45.55

Table 6 – Train, Val and Test Relative Error for CNN with ReLU Activation function

3.5. Training Plots

a. Linear Activation Function

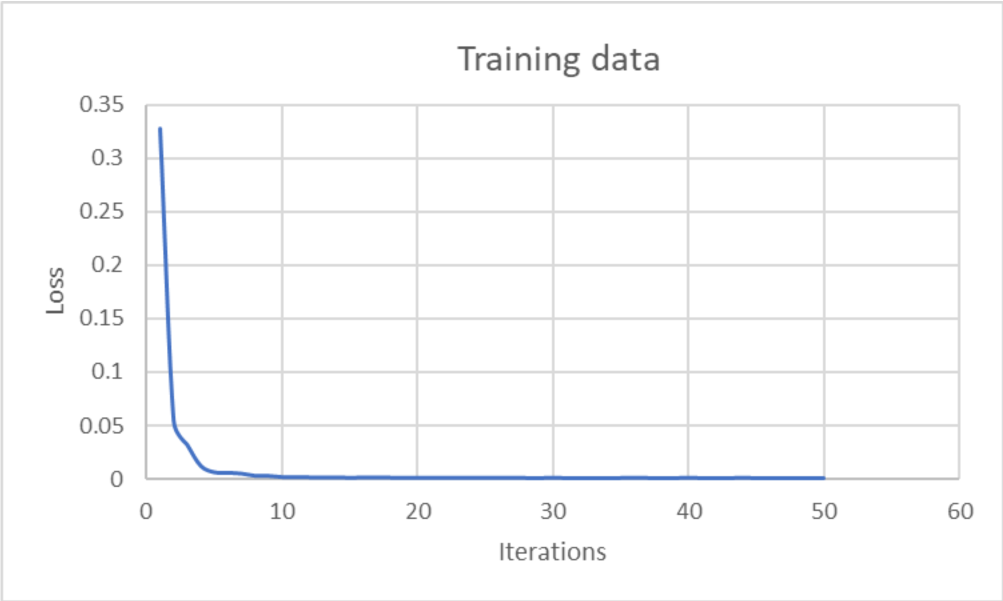

Fig. 4 – Loss v/s Iterations for training data

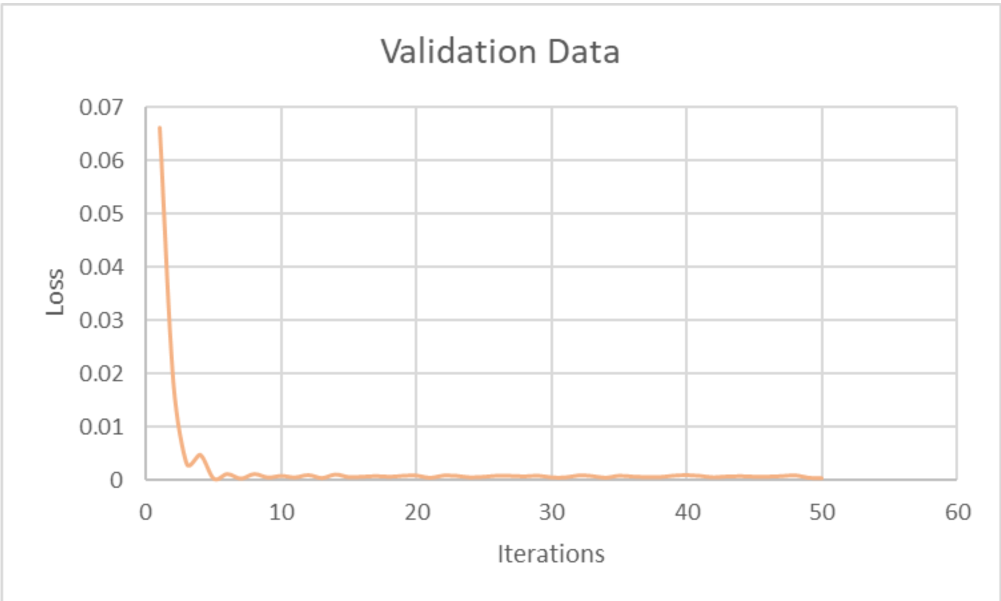

Fig. 5 – Loss v/s Iterations for validation data

Fig. 6 - Relative error v/s Iterations for training data

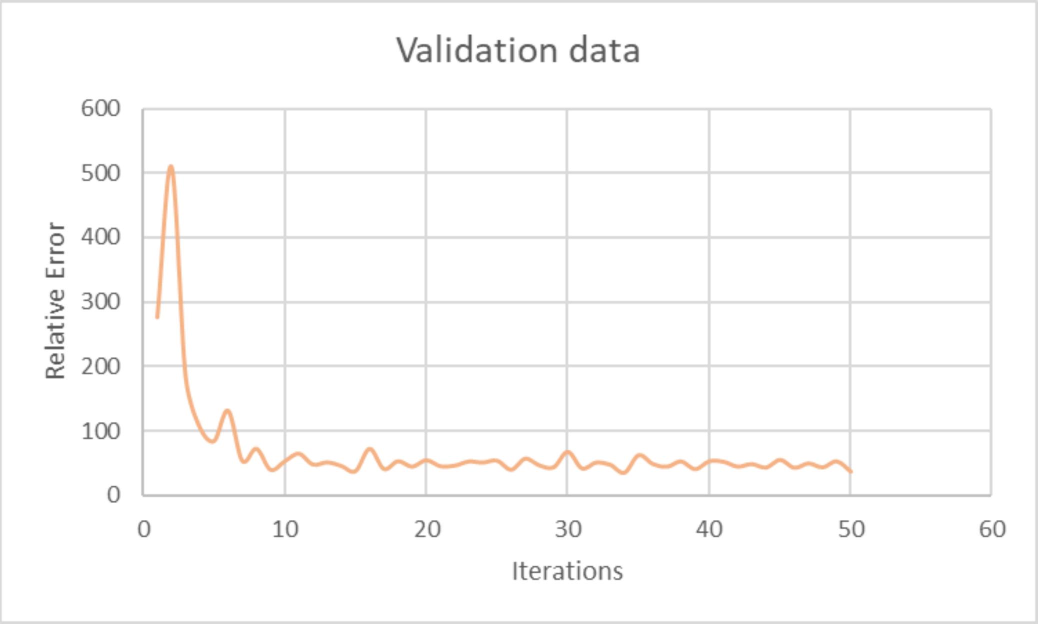

Fig. 7 – Relative error v/s Iterations for validation data

b. ReLU Activation function

Fig. 8 – Loss v/s Iterations for training data

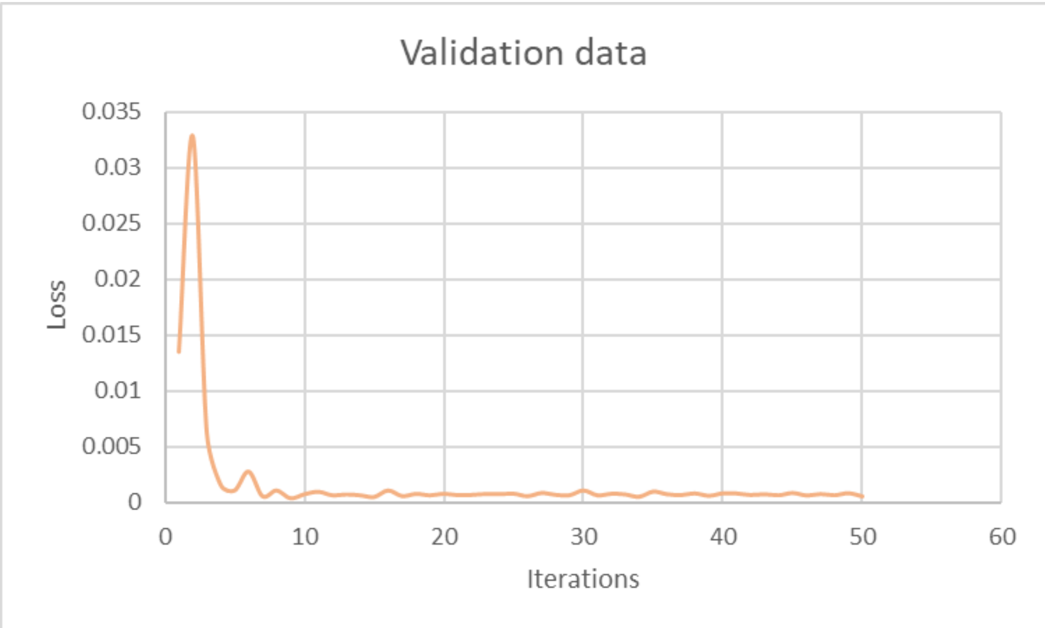

Fig. 9 – Loss v/s Iterations for validation data

Fig. 10 – Relative error v/s Iterations for training data

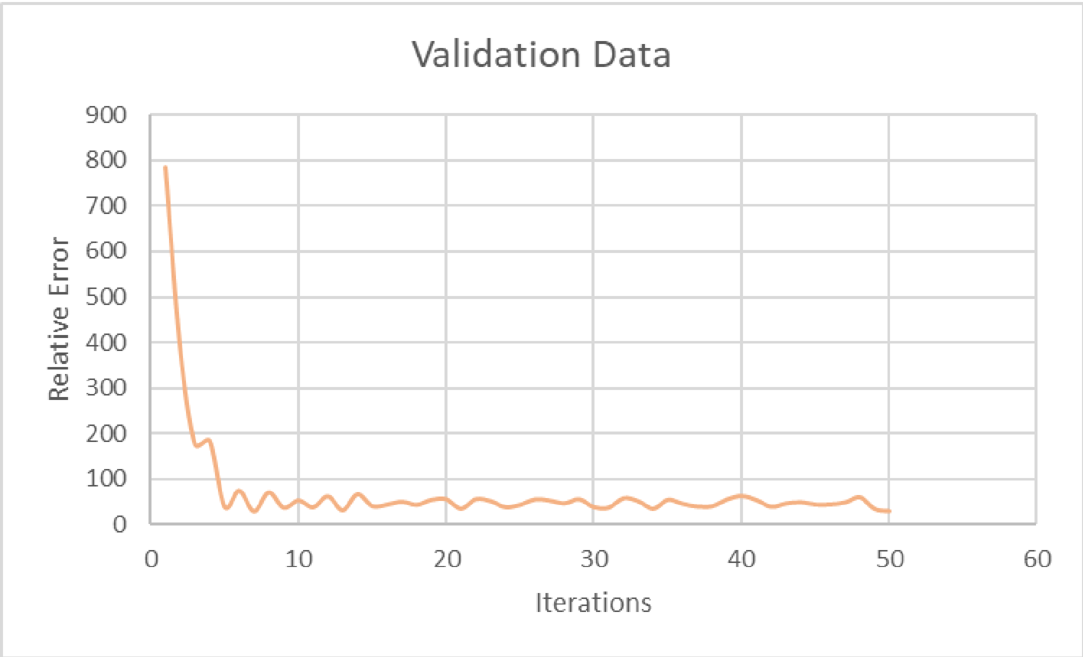

Fig. 11 – Relative error v/s Iterations for validation data

3.6. Results

In this section, we highlight all the details of the dataset, the architecture used, hyperparameter optimization and the final resultant model that we have to predict effective diffusivity of porous media.

Dataset contains binary images in the form of csv file as input and diffusivity values as targets. The targets are normalized to transform diffusivity to effective diffusivity and the data is then split into train, validation and test data with each being 90%, 10% and 10% respectively. Since the dataset contains only 300 images with rather simple features, we do not go for pretrained SOTA architectures like ResNet, VGG, EfficientNet, etc. and we rather stick to a basic 2-layer convolutional neural network to train the model.

We treat all the functionalities of this network like kernel size, number of filters, padding, activation function, pool size, learning rate, etc. as hyperparameters and we tune this set of hyperparameters to get the best neural network for the given data. As a part of hyperparameter tuning, we train close to 900 different 2-layer networks varying the parameters of the CNN and we finalize 2 models, one with a Linear Activation function and other one with a ReLU activation function. We get superior results with Linear Activation function but with more complex features, ReLU may be quite useful and hence we keep two models to predict effective diffusivity. We also observe that a larger filter (4x4, 5x5) provides us with better results as compared to a smaller filter (3x3), likely because the narrow filters cannot capture some important features spanning moderate to large numbers of pixels. Similaryly, all other hyperparameters are chosen and varied.

With Linear Activation function, we get a relative error of 30.73% on validation dataset and a relative error of 39.71% on test dataset as specified in Table 4. With ReLU Activation function, we get a relative error of 36.39% on validation dataset and a relative error of 45.55% on test dataset as specified in Table 6. With these results in hand, we have made significant improvement in Relative Error and we further try to improve the results by using more suited neural network for the given data that may be able to capture the features more significantly and produce better results. We will further try to train a neural network with porosity values that will ingest a physical viewpoint to the whole neural network and may be helpful in further improving the results.

4. Future Work

4.1. Porosity Informed CNN

The key features determining the effective diffusivity of a porous structure are extracted through the convolutional layers and these features are mostly connected with the input images locally. Therefore, global features or features spanning large scale may not be effectively extracted using the CNN, which may compromise the predictive power of the CNN. Therefore, it may be useful to directly introduce physical parameters describing these features into the CNN model to improve its performance.

4.2. Pre-processed pore structures as input

CNNs exhibits relatively large error for porous samples with very small diffusivity ($De < 0.1$). This is closely related to the more complex transport behaviour in porous media with very small diffusivities: in these media, the diffusion pathways are tortuous and there exist many trapped pores and dead-end paths. Since CNN models may not effectively extract features of these complicated structure spanning relatively large length scales using filters with small spatial extent, they do not perform well for such porous media. Hence, we would like to explore the possibility of improving CNN prediction by processing the images of porous structures to remove dead-end and trapped pore spaces.

5. References

1. Predicting Effective Diffusivity of Porous Media from Images by Deep Learning (nature.com)
2. Towards the digitalization of porous energy materials: evolution of digital approaches for microstructural design - Energy & Environmental Science (RSC Publishing) DOI:10.1039/D1EE00398D
3. Wu, J., Yin, X. & Xiao, H. Seeing permeability from images: fast prediction with convolutional neural networks. *Science Bulletin* **63**, 1215–1222 (2018)
4. Code reference - aurorlhc/property_test: Predicting Young's Modulus of porous materials using CNN (github.com)

APPENDIX

Learning Rate	Kernel size	Stride	Pool size	Padding	No. of filters in 2 layers	Train RE	Val RE	Test RE
0.01	2x2	2x2	2x2	Same	8,16	48.43	44.00	48.44
0.01	4x4	4x4	2x2	Same	16,32	50.29	46.98	49.52
0.001	3x3	3x3	2x2	Valid	8,16	49.32	48.52	45.46
0.0001	4x4	2x2	3x3	Valid	32,64	47.31	92.66	97.01

Table 7 – Effect of changing hyperparameters on train, validation and test relative errors

The results for 900 valid combinations of hyperparameters has been summarized in Results_Linear and Results_ReLU. All the models are trained using the same train, validation and test dataset. Hyperparameter tuning is one of the most important aspects of developing a neural network or any machine learning model. Hyperparameters are cross validated using validation dataset. The combination of hyperparameters that gives us the lowest relative error on the validation dataset is considered to be the best model. The best results for our dataset have been summarized in Table 3 – Table 6 above.