Title:
Design of Porous Structures

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Introduction:
A porous medium is a solid material that consists of uniformly or randomly distributed pores or voids. Porous materials have a wide range of applications such as heat exchangers, energy damping equipment, filtration, sound absorption, artificial skin and scaffolds. Parameters affecting the geometry and topology of porous structures are pore size, pore shape, pore distribution, pore interconnectivity, porosity, specific surface area and strut thickness. Physical properties of interest to applications include permeability, effective thermal conductivity, compressive strength, electrical conductivity, damping capacity and tortuosity. Design and modelling of porous structures is very complex in nature, which virtually rules out the possibility of analytical approaches to design porous structures given desired properties. Experimentation and in recent years, computer aided techniques (i.e. numerical simulation) are utilized to find optimum porous materials for any given application. Yet, both techniques have shown cost-efficiency disadvantages. Topology optimization offers a distinctive benefit of determining a feasible solution for this problem; however, it has an inherent drawback in terms of computational cost because of many design variables and iterations [7]. Optimization algorithms, like the ones used in machine learning, have proven to be an alternative tool when dealing with large data and finding an empirical model in the absence of a physics based one. Even though the use of machine learning is a well-established technique in other fields, its application in engineering applications is relatively new. In this paper we explore the use of machine learning to obtain a model to predict geometry of porous material for prescribed physical properties.

A numerically simulated data set is employed by a Machine Learning technique in order to establish a relationship between the input parameters (Permeability and Effective Thermal Conductivity) and the output parameters (Porosity, Number of Pores, Pore Shape). The results obtained from the analyses are compared with simulated results from computational models. To maintain right balance of properties needed for specific engineering application, multifunctional porous materials are necessary along with the correct selection of appropriate porous structure geometry.

Literature Review:
In literature, different ways have been attempted to represent and model porous structure like unit cell method, where a 'unit cell' refers to a representative pore structure of the inner architecture of the porous object [13]. A design strategy has been developed for eventual fabrication of porous titanium structures with periodic cellular structures targeted to biomedical applications [9]. Re-creating porous structures from actual micro-CT images [10] have been attempted. A representation of model density and porosity based on stochastic geometry was introduced and used to create CSG based models of heterogeneous objects [12]. Limitations of these methods include difficulty in modelling porous structures with intricate shapes, resulting in huge file size of a CAD model and, need for an existing

porous object for image reconstruction methods. Boolean operations in stochastic geometry approach consume more time and computing capacity. There are no formal methods to represent a 3D porous structure. Most importantly, there is no predictive control over geometrical properties in any these methods. Convolutional Neural Networks (CNN) have been used to provide a quick assessment of 2D slices of rock images by estimating permeability-correlated properties like porosity, average pore size, and coordination number from greyscale micro-CT images [2]. Synthesizing a porous structure from a given set of desired physical attributes/properties has not been attempted.

Problem Statement and Methodology:

Given a porous object, methods to characterize and extract the physical properties using experimental techniques is well established. But given the properties, methods to arrive at the appropriate porous structure is not known. Proper correlation between the physical properties and geometrical parameters will lead us to parameterize porous structures easily. Complicated and conflicting relations between geometrical parameters and physical properties make it difficult to solve this problem. Our eventual objective is to develop a CAD based representation technique based on geometric and topological modelling approaches to develop complex pore structures based on their field of application thereby ensuring feasibility of manufacturing of developed models by additive manufacturing techniques. Our main objectives are

- A tool to model and represent porous structures given functional characteristics prescribed by the designer
- Derive a CAD model of the porous structure that can be used to realise it through additive manufacturing

In this paper the focus is on the first objective.

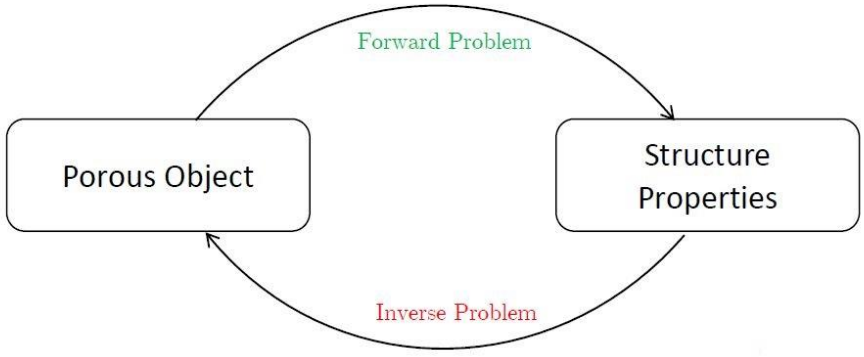

Figure 1: Forward Problem and Inverse Problem

Forward Problem: Characterization of physical properties of porous object
Inverse Problem: Design of porous structure for prescribed physical properties

A dataset of 213 CAD models of porous structures were created using Grasshopper [6], a visual programming language and environment that runs within the Rhinoceros 3D CAD application [11]. The corresponding physical properties extracted using COMSOL Multiphysics [5] are targets for the training deep learning model. TensorFlow [14], end-to-end open source platform for machine learning is used as our deep learning architecture. Keras [8], an open source neural network library that runs on top of TensorFlow is utilized to train our deep learning model. Geometrical parameters like porosity, number

of pores, shapes of pores are fed to a deep learning model as target and computed physical properties such as Permeability and Effective thermal conductivity as an input for the training stage of the model.

The effective thermal conductivity k_e is calculated as a function of thermal conductivity of solid phase k_s and of fluid phase k_f and volume content of each phase or porosity. The mechanism of heat transfer in porous materials is complicated by the irregularity of the internal structure and heat is propagated by thermal conduction through the solid phase and fluid phase, radiation between solid particles and convection in the fluid phase.

Permeability is the property of a porous medium that describes its ability to allow fluid to pass through it. The basic law governing the flow of fluids through porous media is Darcy's Law which establishes the relation between the pressure drop and flow rate.

$$Q = \frac{\kappa A(p_b - p_a)}{\mu L} \tag{1}$$

Where, Q is Volume flow rate, κ is Permeability, A the cross-sectional area, μ the dynamic viscosity of the fluid, p is the Pressure and L is length over which the pressure drop is taking place.

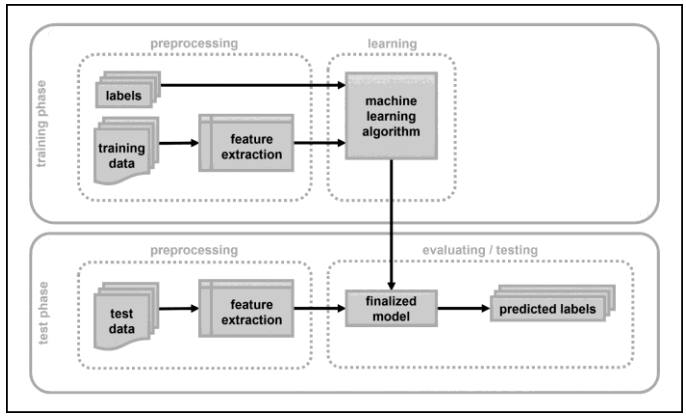

Fig. 2: Overview of the Workflow of Machine Learning Process

Sequential modelling is used in Keras. First inputs and targets are transformed using MinMaxScalar with feature range of -1 to 1. The network consists of one hidden layer of 10 neurons with the Rectified Linear Unit (RELU) activation function [1]. Target Layer is passed through 'Linear' activation function because our problem is a regression problem. We use mean square error to calculate the error between calculated and predicted values from the network. After calculating the error, we use RMSPROP optimizer [4] to update the network weights and biases of layer. Train_test split approach is used for cross validation with 80% of the data for training and 20% for testing. Batch size of 30 is kept and 500 epochs are run. An epoch of training is completed when the whole training dataset has been fed into deep neural network.

Predicting shape of the pore is a multi-class classification problem. One hot encoding is performed on data to perform the multiclass classification. Fully connected network with one hidden layer that contains 8 neurons with RELU activation function and target layer is passed through 'Softmax' [3]. Adam gradient descent optimization algorithm [4] with a logarithmic loss function (categorical_crossentropy) is used to train the network. K- fold cross validation is used.

In the above analysis we have built two different deep learning architectures for regression problem and classification problem. Regression analysis is used to predict porosity and number of pores and multi-class classification is used to predict the shape of the pores. Combining both regression and classification problems in a single deep learning is complicated because the target layer will contain both the outputs (i.e. regression and classification) and assigning different activation functions for these targets is difficult.

Results and Discussion:
Supervised machine learning algorithm (linear regression) was performed in order to predict geometric parameters of porous structures with physical properties based on the application being inputs to the learning algorithm

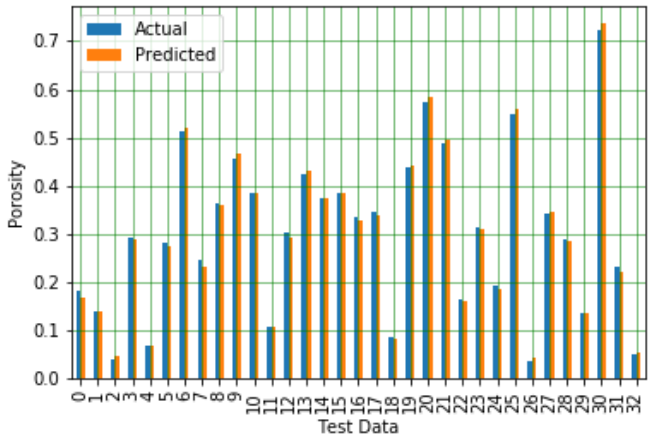

Fig. 3: Plot of porosity for actual vs predicted values.

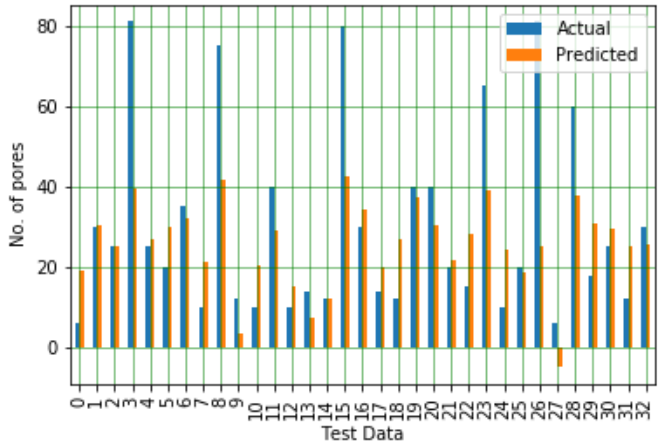

Fig. 4: Plot of number of pores for actual vs predicted values.

Results in figures 3 and 4 show that deep neural network predictions are very close to the actual values and from figures 5 and 6 we can see that the deep neural network accuracy improves, and model loss reduces as more training epochs are completed and the neural network weights and bias are updated. The error between predictions and the actual values for porosity is very less compared to the number of pores. Mean squared error (MSE) for porosity and permeability are approximately 0.003 and 190 respectively.

From figure 3 and 4 we can see that the error for predicting porosity is very low compared to predicted values of number of pores because effective thermal conductivity is strongly related to porosity, which is in agreement with the literature. Permeability of porous structures is usually expressed as function of interconnected pore system such as porosity and tortuosity. We have considered one of the most widely accepted and simplest models for the permeability-porosity relationship, Kozeny-Carman model (equation 1), hence the prediction of porosity is performed with least error. As effective

thermal conductivity and permeability are input and porosity is one of the targets, the deep neural network can exactly correlate the input-target relationship.

But the error in the predictions of number of pores is large because the correlation between effective thermal conductivity and permeability with number of pores is not exactly known. It is also possible that the deep learning model may require more data to make the estimations of number of pores with minimum error.

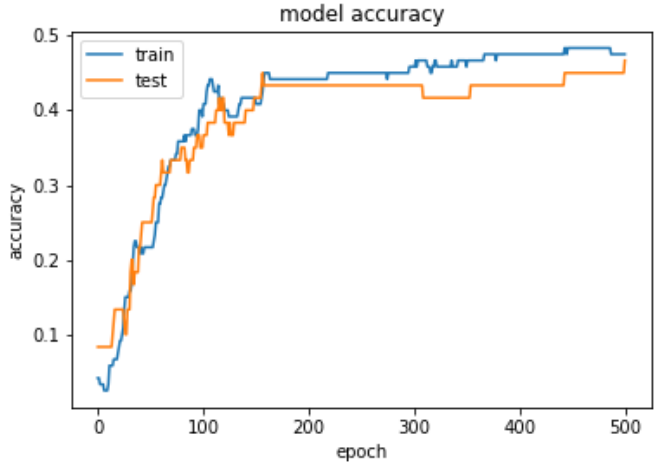

Fig. 5: Model accuracy during training and testing.

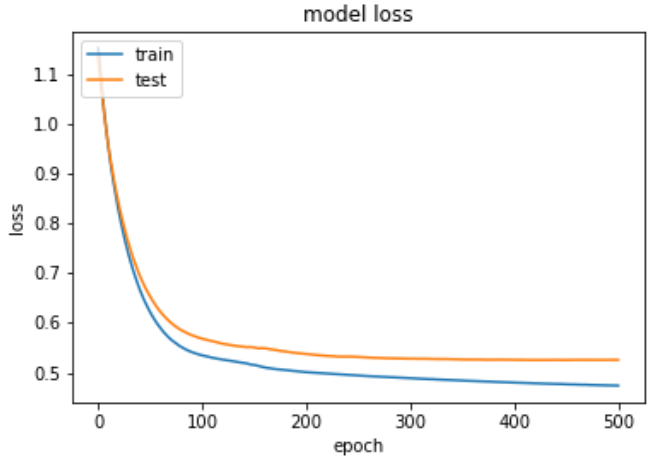

Fig. 6: Average epoch loss during training and testing.

K-fold cross validation with 10 folds is used. Accuracy is 49.21% of mean and 9.75% of standard deviation.

The datasets used in this study are small compared to the number used typically in deep learning. As availability of data is likely to be restricted, one direction to explore is how convergence in deep learning can be enhanced for relatively smaller data sets. As mentioned earlier the data regarding physical properties were obtain through numerical computation (COMSOL Multiphysics). While these values do represent true values in present practice, it is necessary to validate the results through actual prototyping of the porous structures and testing.

Conclusion:
Regression and multi-class classification machine learning models are used for estimating geometrical parameters of porous structure given physical properties based on application mentioned is presented in this paper. A dataset was created with physical properties of porous structure as input and geometrical parameters as targets. The physical properties considered for analysis are effective thermal conductivity and permeability and geometrical parameters are porosity, number of pores and pore shape. Keras with TensorFlow backend is utilized to develop deep learning network. The error between predictions and the actual values for porosity is very less compared to the number of pores. Mean squared error (MSE) for porosity and permeability are approximately 0.003 and 190 respectively. For predictions of pore shape the accuracy is 49.21% of mean and 9.75% of standard deviation. Future work is to include some more physical properties like compressive strength, acoustic properties and electrical properties for inputs and strut thickness, spatial distribution of pores, specific surface area and tortuosity. Larger dataset will ensure that our algorithm works fine as we are using deep learning architecture.

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