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Design of Porous Structures

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Abstract. Modeling of porous structures is challenging because of the heterogeneity in structure and complex relations between its geometry and physical properties. In this paper, we have used machine learning to define porous structures given the desired physical properties as prescribed by the user. A dataset was created with the physical properties of the 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. The results obtained from the analyses are compared with simulation results from computational models.

Keywords: Porous Structures, Machine Learning, Inverse Problem, 3D Printing
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1 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. The design and modeling of porous structures are very complex, which virtually rules out the possibility of analytical approaches. 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 [13]. Optimization algorithms, like the ones used in machine learning, have proven to be an alternative tool when dealing with lots of 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 the geometry of porous material for prescribed physical properties.

A numerically simulated data set is employed by a Machine Learning technique to establish a relationship between the input parameters (Permeability and Effective Thermal Conductivity) and the output parameters (porosity, number of pores and pore shape). The results obtained from the analyses are compared with simulated results. To maintain the right balance of properties needed for specific engineering applications, multifunctional porous materials are necessary, the correct selection of appropriate porous structure geometry is necessary. CAD models are generated with the obtained geometrical parameters. The results obtained from the analyses are compared with simulation results from computational models.

2 LITERATURE REVIEW

The overall objective of this research is to develop tools automate the realization of a porous structure that meets a specified functional requirement. To the best of our knowledge, this specific objective has not been addressed in the literature so far. Related work in the literature, have been reported in the areas of modeling and representation of porous structures, the relationship between geometry and the physical properties of a porous structure, and the use of data-based techniques to predict properties of a porous structure.

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 [27]. Different polyhedral shapes for modeling scaffolds have been investigated and classified into unit cells and a parametric library of scaffold structures created [7],[8]. A design strategy has been developed for the eventual fabrication of porous titanium structures with periodic cellular structures targeted to biomedical applications [19]. Triply periodic minimal surface TPMS, which can effectively describe the surface morphology and pore size distribution of the bone structure has also been proposed as unit cells for modeling bone scaffold [26]. The limitations of these methods are that natural and complicated structures cannot be modeled easily and typically result in huge file sizes. These cause difficulties during conversion to STL files for fabricating them [18]. Models of porous objects have been constructed from images obtained through computed tomography (CT) and magnetic resonance imaging (MRI). Accurate models of micro-scale scaffolds have been generated from micro-CT. This model is manufactured employing 3D additive manufacturing process from biocompatible materials [20]. The drawbacks of image reconstruction methods are that an existing porous object is required and there is no control over geometrical properties [30].

Stochastic geometry methods [28] model the internal shape parameters as a stochastic process. A representation of model density and porosity based in stochastic geometry was introduced and used to create CSG based models of heterogeneous objects [23]. Monte Carlo simulation (i.e., stochastic processes) is used to create a set of layered point-clouds so that the solid models generated from the point-clouds exhibit randomly distributed porous structures and finally physical models were built from the solid models using the commercially available additive manufacturing facilities. Stochastic geometry method is good to realize the porosity, pore size, and pore distribution of porous structures [24]. This method has a strong representation ability, while the Boolean operation is a time-consuming process and adds heavy burdens to computer processing. Voronoi tessellation/Delaunay triangulation methods in which a pore is generated in each Voronoi cell to efficiently design optimized porous solids with good strength to weight ratio has been proposed [32]. While the above efforts focus on building models of porous structures, the models obtained cannot be manipulated to achieve desired physical attributes.

Work has been reported in the literature on predicting or estimating values of physical attributes based on geometric attributes such as pore size, shape, orientations, and concentrations (porosity). Thermal conductivity is determined by Archie's law, whose exponent depends strongly on the shape and orientation of the pores [12]. Effect of the pore shape on the thermal conductivity of porous media is studied [17]. They found that the effect of the pore shape becomes

stronger as the porosity increases and the thermal conductivity for randomly oriented pores takes its maximum value for spherical pores. The influence of pore variation on thermal conductivity of open porous foams was discussed in [25]. Permeability is described by an effective hydraulic pore radius in the porous medium, the fluctuation in local hydraulic pore radii, the length of streamlines, and the fractional volume conducting flow [3]. The effect of volume, surface, curvature, and connectivity on the hydraulic conductivity [15]. Combining parametric finite element models of scaffolds with numerical optimization methods and a computational mechano-regulation model, an optimal scaffold microstructure was modeled taking pores shape, number, and spatial distribution in the account. The optimal dimensions of the pores have been determined for different values of scaffold Young's modulus and compression loading acting on the scaffold upper surface [4]. Combined heat sinking and noise reduction in the same functional volume is reported and thermal-acoustic co-design of 3-D periodic porous foam structures [21]. Porosity and bone surface area are the main factors to control [10]. The focus in this paper is to design a porous structure, that is to arrive at the geometric attributes given specific functional attributes.

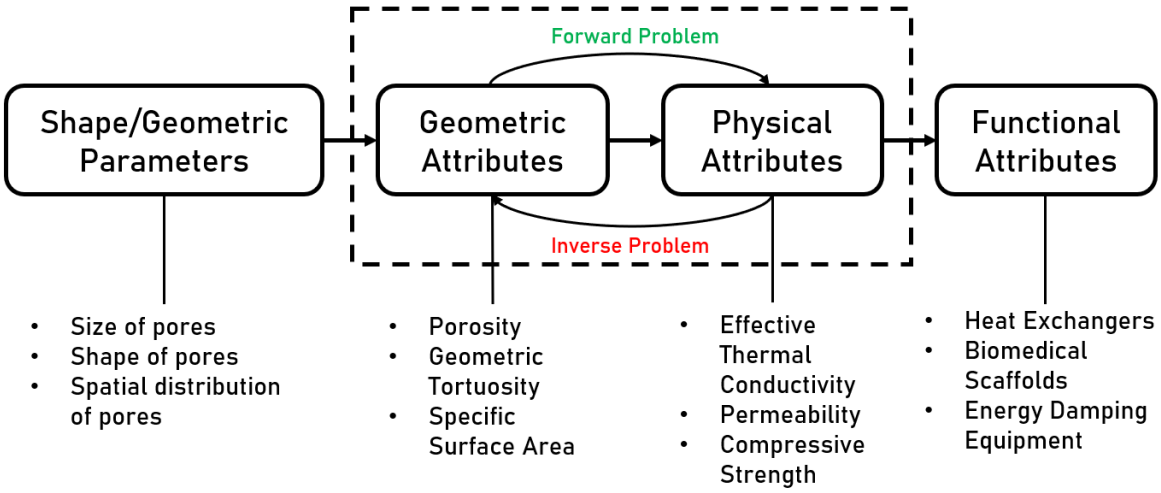
Convolutional Neural Networks (CNN) has been used to provide a quick assessment of 2D slices of rock images by estimating permeability-correlated properties like porosity, average pore size, and coordination number from greyscale micro-CT images [2]. Fast prediction of permeability of porous media from pore-scale images is done using CNN. The CNN-based permeability prediction method is orders of magnitude faster than direct simulations using lattice Boltzmann [31]. Three-dimensional stochastic image reconstruction based on generative adversarial neural networks (GAN) is used to train three-dimensional segmented images [16].

Herein, our objective is to design porous structures based on user-defined physical properties. Machine learning approach is utilized to predict the geometrical parameters of the porous structure given the desired functional properties.

3 PROBLEM STATEMENT AND METHODOLOGY

Given a porous object, methods to characterize and extract the physical properties using experimental techniques are well established. But given the properties, the method to arrive at the appropriate porous structure has not been addressed. 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 objective is to automate is the realization of a porous structure that meets a specified functional requirement. As shown in figure 1, the functional requirement depends on the physical properties (thermal conductivity, permeability, strength) of the structure which in turn depends on geometric attributes of the structure (porosity, the shape of pores). Design/modeling parameters have to be derived from the desired geometric attributes so that a representation or model of the porous structure can be obtained that can then be used to realize a physical embodiment of the porous structure. In this paper, only the estimation of geometric attributes given the desired physical properties has been addressed. A data-driven machine learning-based approach has been proposed for this.

From literature, it is found that porous structures are known for physical properties like permeability, effective thermal conductivity, compressive strength, electrical conductivity, damping capacity, and tortuosity. These structures are governed by geometric parameters like pore size, pore shape, pore distribution, pore interconnectivity, porosity, specific surface area, and strut thickness. Since our aim here is to obtain a model to predict the geometry of porous material for prescribed physical properties. It is very difficult to obtain a relationship between inputs and outputs analytically. Hence machine learning is used to derive such a complicated relationship between inputs and outputs. In this paper, we have considered effective thermal conductivity and permeability as physical properties of porous structures as these are the most important and influential properties in fluid transport and heat transfer applications.

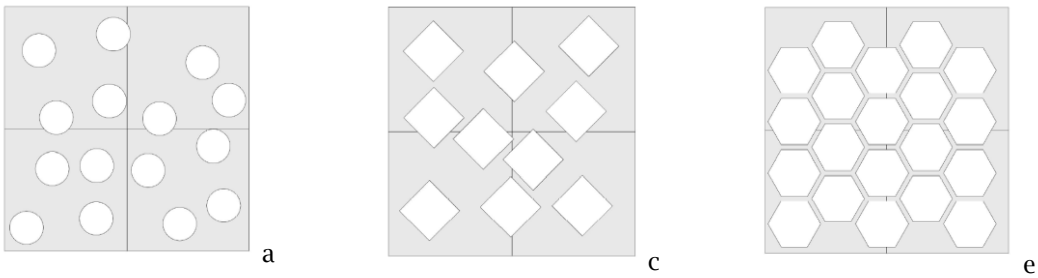


Forward Problem: Characterization of physical properties of a porous object (analysis)
Inverse Problem: Obtain porous structure with prescribed physical properties (design)

Figure 1: Schematic of Design/Analysis of Porous Structures.

A dataset of 213 CAD models of porous structures was created using Grasshopper [11], a visual programming language and environment that runs within the Rhinoceros 3D CAD application [22]. The corresponding physical properties extracted using COMSOL Multiphysics [9] are targets for the training deep learning model. TensorFlow [29], an end-to-end open-source platform for machine learning is used as our deep learning architecture. Keras [14], 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 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.

In our analysis, we have considered open porous structures. Pore with simple geometry (circle, rectangle, and hexagon) of different sizes are extruded on a cube of 100x100x100 mm^3.



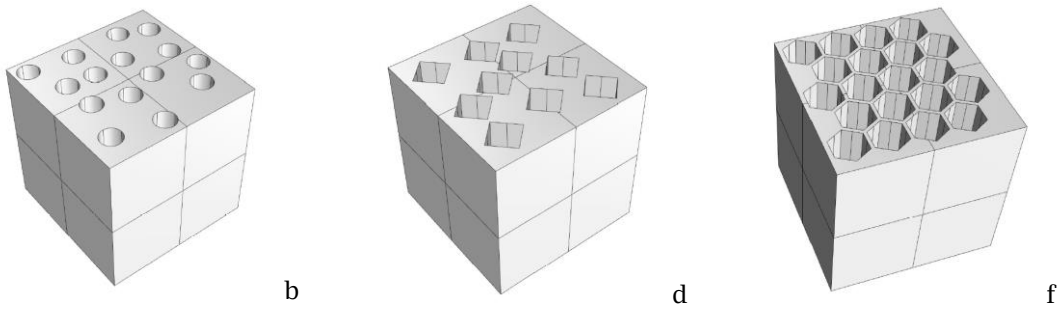


Figure 2: Sample data set of CAD models created in Rhinoceros 3D to extract physical properties in COMSOL Multiphysics (a, b) Circular pore shape, (c, d) Rectangle pore shape, and (e, f) Hexagonal pore shape.

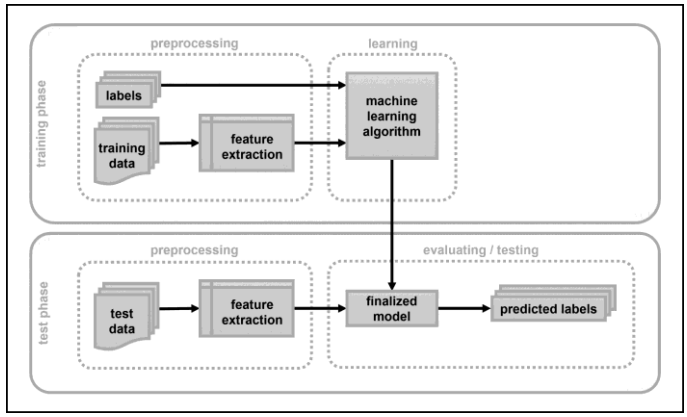


Figure 3: Overview of the Workflow of Machine Learning Process.

Sequential modeling is used in Keras. For predicting porosity and the number of pores, regression analysis is used. First inputs and targets are transformed using MinMaxScalar with a 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]. The target layer is passed through the '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 [6] to update the network weights and biases of the layer. Train_validation_test split approach is used for cross-validation with 60% of the data for training, 20% for validation, 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 a deep neural network.

For predicting the shape of the pore, multi-class classification problem. One hot encoding is performed on data to perform the multiclass classification. A fully connected network with one hidden layer that contains 8 neurons with RELU activation function and target layer is passed through a normalized exponential function ('Softmax' [5]). Adam gradient descent optimization algorithm [6] 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 the regression problem and classification problem. Regression analysis is used to predict porosity and the number of pores and multi-class classification is used to predict the shape of the pores. Combining both regression and classification problems in 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.

4 RESULTS AND DISCUSSION

Supervised machine learning algorithm (linear regression) was performed to predict geometric parameters of porous structures with physical properties based on the application being inputs to the learning algorithm.

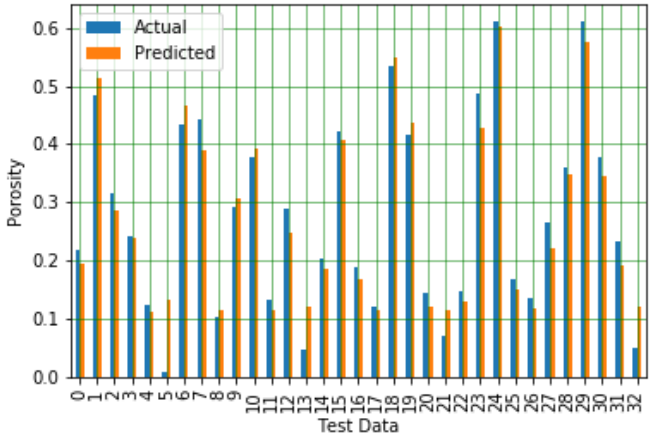


Figure 4: Porosity - actual vs predicted values.

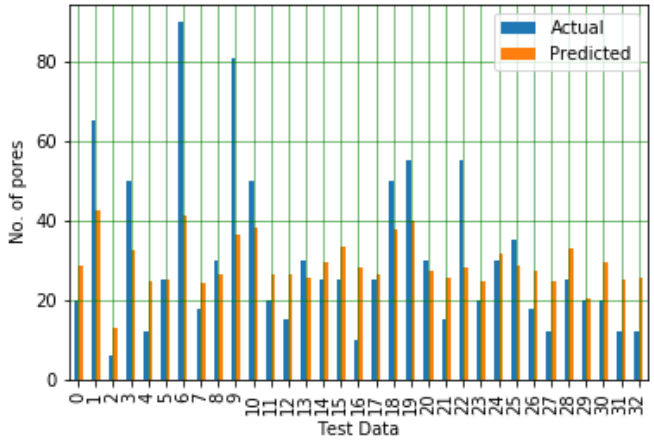


Figure 5: Number of pores - actual vs predicted values.

From figures 4 and 5 deep neural network predictions are very close to the actual values and from figures 6 and 7 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 185 respectively.

From Figures 4 and 5 we can see that the error for predicting porosity is very low compared to predicted values of the 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 a function of interconnected pore systems 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, hence the prediction of porosity is performed with the 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 the number of pores is large because the correlation between effective thermal conductivity and permeability with the 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 the number of pores with less error.

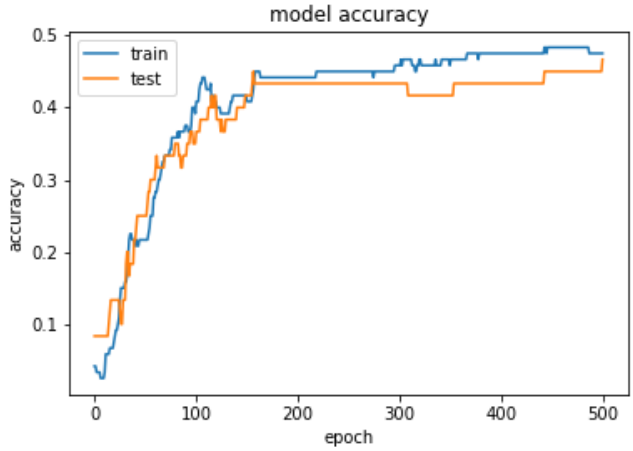


Figure 6: Model accuracy during training and testing.

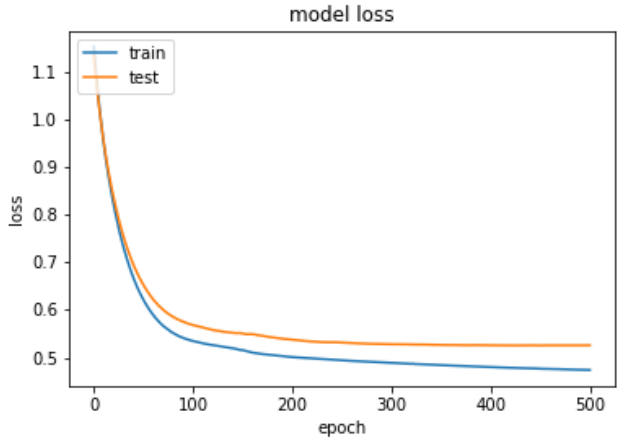


Figure 7: Average epoch loss during training and testing.

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 the 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 obtained 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.

5 CONCLUSIONS

Regression and multi-class classification machine learning models are used for estimating geometrical parameters of porous structure given physical properties based on the application mentioned is presented in this paper. A dataset was created with the physical properties of the 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 a 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 185 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, the spatial distribution of pores, specific surface area, and tortuosity. The larger dataset will ensure that our algorithm works fine as we are using deep learning architecture. Also, it is necessary to validate the present model through physical prototyping of the porous structures using the additive manufacturing process and testing.

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