Can Minkowski tensors of a porous microstructure determine its permeability?

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Abstract

Using the data from a large number of simulations of flow through periodic unit cells containing complex shaped obstacles, we show that the permeability of porous media can be accurately predicted using the Minkowski tensors describing the obstacle shapes. The prediction is achieved by training a deep neural network (DNN). Minkowski tensors have been widely used as generic shape descriptors for many different kinds of two phase systems. Hence, our finding implies that the permeability of a general porous media may also be accurately modeled from available pore-structure information represented as Minkowski tensors. We present the validation of our DNN models for shapes with increasing complexity, decreasing data set size and using the individual Minkowski tensors exclusively. These results prove that Minkowski tensors of the pore microstructure are sufficient to determine the porous permeability, although the functional relationship could be complex to determine.

Key words: Porous media, machine learning, shape description, Minkowski tensors, deep neural network

1. Introduction

The explicit relationship between the porous permeability and the pore-scale geometry of a porous medium has remained an unsolved problem for nearly a century. While the influence of porosity on permeability is very well studied\cite{12, 5, 6}, the effect of the shape of the porous structures itself

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on permeability has remained a challenge. This difficulty is two-fold: (1) shape being an infinite-dimensional quantity is difficult to describe using finite number of parameters (2) the identification of the shape descriptors that are relevant to the permeability of the porous microstructure. In this paper we identify Minkowski Tensors (MTs) \cite{17} as shape descriptors for the porous microstructure by showing that MTs are sufficient to determine its permeability. To demonstrate this, we use the data generated from a large number of computational fluid dynamics (CFD) simulations of flows through 2D periodic porous media (with arbitrarily complex shaped structures in each periodic cell).

Shape, in general, can be represented to any spatial resolution resulting in an infinite dimensional parameter space. Spatial discretizations (like voxel data from tomograms or the points on a reconstructed surface) as well as parametric representations (such as spherical harmonics) of shapes could be used as shape descriptors. While the first class of descriptors is governed by the resolution of observation and, therefore, may require processing of a large amount of data, the latter may not be applicable to general porous structures. Simple representations relevant to flow through porous media, such as the widely popular ‘tortuosity’ \cite{7} or Euler characteristics \cite{16} while being very important and relevant to porous media are insufficient to fully determine permeability. Also these measures require medium-specific experimental observations \cite{11}.

Minkowski Tensors have been introduced in recent times \cite{17} as a shape descriptor for a variety of different complex shaped media such as cellular structures and granular media. In granular media, for example, MTs reveal properties of packings that have been difficult to obtain by any other descriptors \cite{15}. While there is some enthusiasm in relating Minkowski functionals (MTs are a generalization of the functionals) to porous permeability \cite{1}, there is currently no study conclusively showing that MTs determine permeability \cite{16}.

We use 2D periodic domains each containing a complex shape, generated by a random process. Subsequently, we simulate the flow through each of these representative elementary volumes (REVs). In total, we perform CFD simulations for a hundred thousand unique shapes with constant volume (to represent constant porosity across our samples) and for different flow velocities (for Reynolds number less than 1). From the obtained data, we determine the porous permeability for each of the REVs. Additionally, we compute the MTs for each of the shapes in the REVs. Finally, we train
a Deep Neural Network (DNN) model to predict the permeability as a function of the MTs.

The obtained model can predict permeability to high accuracy establishing that knowing the MTs for a given structure is sufficient to determine the porous permeability for at least the considered class of porous media. Owing to the fact that MTs can be used to represent arbitrary shapes, showing that MTs can sufficiently determine porous permeability even for a certain class of porous media provides us with the confidence to hypothesize that MTs can in principle determine permeability in a general sense. In this paper we present the CFD simulation setup used for generating data, the description of the MTs used as attributes for the DNN training and the set up of the DNN used to obtain the model for the porous permeability. Further, we present the results for shapes of increasing complexity and discuss the individual prediction capacity of each of the MTs. The data and the DNN parameters are provided as supplementary material to enable further exploration by the readers.

2. Shape generation and flow simulation

In order to test if the MTs can sufficiently predict porous permeability, we have to consider a system which is complex enough, but computationally not too challenging, so that obtaining a large data set is possible in a reasonable period of time. Also the system we use should account for shape effects that are beyond the obvious dependence of permeability on the porosity. Considering these factors we generate square 2D domains with periodic boundary conditions on all 4 sides containing a complex simply connected arbitrary shaped obstacle. The obstacle is assigned no slip wall boundary condition. This domain thus forms the REV of the porous media and each shape corresponds to a different porous media.

The shapes are generated using a method illustrated in Fig. 1. Ten points are spawned at equal angular intervals with randomly chosen radial coordinates. A Fourier parametric curve is fitted to these points using a least square minimization algorithm. Similar approaches are widely used in reconstructing arbitrary non-convex shapes [20, 21]. The parametric representation of the shape is of the form:
\[ x(\theta) = \frac{1}{2} X_0 \sum_{i=0}^{m} X^c_i \cos(i\theta) + X^s_i \sin(i\theta) \] (1)

\[ y(\theta) = \frac{1}{2} Y_0 \sum_{i=0}^{m} Y^c_i \cos(i\theta) + Y^s_i \sin(i\theta). \] (2)

For \( \theta \in [0, 2\pi) \), \( x \) and \( y \) describe a shape of order \( m \). The coefficients \( X_0/2 \) and \( Y_0/2 \) give the coordinates of the centroid of a shape. The volume of a given shape can be computed by the formula:

\[ A = \int_{0}^{2\pi} yx' \, d\theta. \] (3)

where \( x' = dx/d\theta \). The shapes are then scaled to a value of 0.5 (to keep the porosity fixed, \( \phi = 0.5 \)) and the centroid \((X_0/2, Y_0/2)\) translated to the center of the unit square domain. Shapes with spikes, self intersections and those with regions outside of the square are eliminated. Different values for \( m \), namely 1, 2 and 3, are considered, and for each of these orders \((m)\), 100,000 shapes are generated. For \( m = 1 \) only ellipses are generated, while higher values of \( m \) results in increasingly complex shapes. Figure 1 shows shapes of increasing order generated with the same set of generator points (positioned at equal \( \theta \) intervals but at random radial locations).

The flow through each of the REVs is then simulated with the Gerris flow solver [14] employing the finite volume method (FVM). This software was chosen because it uses a quadtree mesh for which adaptive resolution can be employed eliminating the need for additional meshing or pre-processing difficulties. For each REV, three different pressure gradients were applied to drive the flow. While its magnitude was varied, the direction of the pressure gradient was fixed. The largest pressure gradient was chosen such that the corresponding Reynolds number \((Re = \rho Ur/\mu\), where \( r \) is radius of the circle of equal area, \( U \) is the superficial velocity and \( \rho \) and \( \mu \) are the density and viscosity of the fluid\) is 1. We, therefore, expect the flow regime not to deviate substantially from the Darcy regime. For each REV, the following applies according to Darcy’s equation for porosity:

\[ -\frac{dp}{d\rho} = \frac{\mu}{K} U \] (4)
Here $\frac{dp}{dx}$ is the applied pressure gradient in the $x$-direction, $U$ is the obtained superficial velocity in $x$-direction, $\mu$ is the viscosity, and $K$ is the permeability (assuming an isotropic porous medium). For each REV, we fit a 2nd order polynomial to relate the pressure gradient, $\frac{dp}{dx}$, to the the superficial velocity, $U$. The slope of this curve at the origin, gives us the coefficient of the linear term in $U$, which according to Eq. 4 is $\mu/K$. As the viscosity, $\mu$, is known, the value of $K$ can computed for each REV.

Figure 2 shows four example shapes from the dataset including the extreme cases, i.e., the most permeable REV (A) as well as the least permeable REV (D). The plot on the left shows the data points and the polynomial fit to this data whose slope at the origin is used to compute $K$.

In Fig. 3 we show the distribution of the permeability values for each considered order, $m$. As $m$ increases, we observe an increasing number of shapes for which permeability drops to zero. This is because the probability of a shape blocking the flow increases with its complexity. This is apparently a truncated normal distribution of permeability values. The permeability values of a periodic arrangement of circles in a square pattern is marked for
Figure 2: Flow through four exemplary shapes of order \( m = 2 \). (A) and (D) correspond to the shapes with maximum and minimum permeability in the dataset, respectively. Also an analytical result [14] for an infinite arrangement of circles of porosity 0.5 in a square pattern is marked using dashed lines in the figure for comparison.

3. **Minkowski Tensors**

Minkowski tensors are generalizations of the Minkowski functionals and can represent any motion covariant shape [17, 11]. Four linearly independent Minkowski tensors can be defined for two spatial dimensions and six for three spatial dimensions. Our study includes only two dimensional analysis. The
corresponding MTs are defined as follows:

\[
W^{2,0}_0 = \int_K \mathbf{r} \otimes \mathbf{r} \, dA \\
W^{2,0}_1 = \frac{1}{2} \int_{\partial K} \mathbf{r} \otimes \mathbf{r} \, dr \\
W^{2,0}_2 = \frac{1}{2} \int_{\partial K} \kappa(r) \mathbf{r} \otimes \mathbf{r} \, dr \\
W^{0,2}_1 = \frac{1}{2} \int_{\partial K} \mathbf{n} \otimes \mathbf{n} \, dr.
\]

Here, \( K \) represents the area chosen for integration and \( \partial K \) represents the boundary of the region \( K \). The vectors \( \mathbf{r} \) and \( \mathbf{n} \) are the position and the unit normal vector at the surface, respectively. Curvature at a point on the surface is denoted by \( \kappa \). Since the shapes we consider have an analytical description, the MTs can be computed analytically. Alternately, the MTs
can be computed numerically using the open source software Papaya \cite{9}. In this work, we follow the latter approach.

Each MT is a symmetric, two-dimensional, $2^{nd}$ order tensor and, thus, contains 3 independent scalar values. For the purpose of building the DNN model we could directly use these elements as the features for the training. However, to provide physical inspiration, we use the Eigen values as well as the elements of the Eigen vectors as training features. This results in six features (scalar values) per MT, making a total to 24 features. In the following section, we discuss the set up of the DNN and its training process.

4. Training the DNN

Beyond the obvious dependency between permeability and porosity, further dependence of permeability on higher order shape effects have been a subject of intense research \cite{3, 19, 18, 13, 8}. The goal is to identify a shape descriptor that can sufficiently determine permeability. It is clear that the functional relationship between a descriptor and the permeability may not be mathematically simple, given the volumes of research undertaken in this area. Therefore, it may be a sensible approach to use today’s data science tools to this end. That is to answer the question if some functional relationship exists between the Minkowski tensors of a porous microstructure and its permeability. As described in the previous section, we consider the Eigen values and Eigen vector elements of the 4 Minkowski tensors forming a 24 dimensional feature space. This could be reduced based on symmetry arguments. However we chose to use the Eigen values and vectors to motivate physical interpretations of the MTs for future research, and for the readers to interpret in case they use the data provided as supplementary material.

The DNN comprises several layers of nodes. Each node is a computational unit that magnifies an input signal $x_N$ by a weight $W$, offsets it by a bias $b$, and finally applies an activation function to it. A node is loosely modeled based on a biological neuron which is activated when a stimuli beyond a certain threshold is applied. The input data applied as a signal is first forward propagated through the arrangement of nodes (in several layers) using random guess values for $W$’s and $b$’s. The final output value is then compared with the expected permeability value $K$ corresponding to the given MTs. The error w. r. t the actual $K$ value is estimated by a loss function, which we have chosen to be the $L_2$ norm of the difference between the prediction and the actual values of $K$. A gradient descent algorithm is then applied to
propagate back a modification to the weights and biases \[10\]. The process is repeated through several iterations called *epochs* in the machine learning parlance. Neural network implementations are available today in a wide variety of open source softwares. We have chosen the *Keras* library with a *TensorFlow* backend for our purpose.

The available dataset is split into a *training set* and a *test set*. While the training set is used to minimize the loss function, the test set is only used to verify if the fitted model performs well. In such an exercise it is important to check if the error in the test set and that in the training set proceed at the same rate as the model converges. A decrease in error in the training set at a higher rate than the error in the test set would mean that the model *overfits* the training data and, therefore, would perform poorly on any data outside the training set. For a successful model, a number of parameters and choices are at the users’ discretion. Considerable effort is required to *babysit* the training model until an error convergence without overfitting is obtained. When the underlying functional relationship between the features and the output is a simple one, the training of the DNN is easier than if the relationship is more complex. Our choice of the activation function, the layer architecture and other options are tabulated in the Appendix section of this paper. An example script in the Python language is also provided as supplemental material.

We show, in Fig. 4, that the model we trained can determine $K$ to a high degree of accuracy: within 6\% error compared to the total variance in the permeability values (see Fig. 3). It is, of course, possible that a better set of parameters exist. Such parameters could reveal that MTs could predict $K$ to an even higher accuracy. We leave this to the interested reader to experiment with, as we provide the dataset and the scripts we have used for training the model. However, we have arrived at accuracy levels that are satisfactory to make the assertion that MTs are sufficient to relate the effects of shape (beyond porosity) to the permeability. Previous studies in relating Minkowski Tensors to permeability have pointed out that this relationship may not be a simple one to determine [1]. A DNN is able to learn such complex relationships from available data and, therefore, it is an ideal tool for this problem. In Fig. 4 as the order of complexity of the shape, $m$, increases, the same DNN is unable to train with the same accuracy. However, the overall accuracy is still high enough for practical purposes and may be improved by tweaking the DNN architecture. We have maintained the same DNN parameters for the sake uniformity across datasets.
In other applications using MTs, there have been difficulties in relating the higher order MTs to physical insights [15], raising the question whether these higher order measures have practical significance. In order to show that all the MTs contribute to the model’s prediction, in Fig. 5, we present training results where only one MT is used at a time (6 features) considering the dataset for \( m = 2 \). Further, for the Y-axis, the same data and normalization approach were used as in Fig. 4b. Clearly all four MTs are independently able to predict the permeability to great accuracy and, thus, contribute to the model. The first and second Minkowski Tensors (Eq. 5 and 6), which hold information about the volume moments and the surface orientation, seem to contribute slightly less to the permeability than the MTs in Eq. 8 which contain information about the local curvatures of the shapes. Thus, information contained in other well known measures such as tortuosity [11] is clearly contained also in the description of the porous microstructure using MTs.

It may be a practically worthwhile question to ask whether a large amount of data may always be required for a successful permeability prediction model. To answer this question we perform the training process with different train-
Figure 5: Training and validation of the DNN with different Minkowski tensors used exclusively as features.

We have demonstrated that the answer to the titular question whether Minkowski Tensors of a porous microstructure can be related exclusively to the permeability of the medium is a ‘yes.’ We have generated a large enough dataset of complex shapes of constant porosity with different orders of complexity and performed CFD simulations of flows through REVs containing...
these non-convex simply connected shapes. We trained a DNN model using this simulated data, validated the model, and demonstrated its accuracy for different shape complexity and for different dataset sizes. Accurate prediction results from even a small number of shapes available for training the model. This indicates that also computationally more challenging systems can be investigated following the procedure outlined above.

Physically, these shapes may be seen as representing cross sections of fibrous porous media. However, the motivation to the above exercise has been to identify a simple system where a data experiment relating the MTs to the permeability may be conducted. Our results show that Minkowski tensors are sufficient descriptors of the pore microstructure, in order to determine its permeability. This result leads us to hypothesize that the same may be true for much larger scale systems in three dimensions and involving non-uniform porous microstructure. Further investigations into anisotropic porous media, where the tensorial nature of permeability is important, are also worth pursuing.
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