Prediction of 3D mass transport properties from 2D data using convolutional neural networks

Background

We use both statistical methods and machine learning to understand the relationship between the structure/geometry of porous materials and their mass transport properties, i.e. diffusive transport and fluid flow. In a recent project, we generated a large number of virtual materials structures and computed diffusivity and fluid permeability using lattice Boltzmann methods. The data set consists of 90,000 binary 3D arrays of size 192^3 and the corresponding computed properties, to our knowledge the largest dataset ever of this kind. We used both artificial neural networks (ANNs) and 3D convolutional neural networks (CNNs) to perform nonlinear regression and predict the mass transport properties with high accuracy.

However, in many practical cases, only 2D data is available. Therefore, it is of interest to develop methods for prediction of 3D properties using only 2D data, e. g. a single slice of the 3D arrays.

Aim

The purpose of the proposed MSc project is to develop methods for prediction of 3D mass transport properties from 2D data using 2D CNNs (and/or possibly other machine learning-based regression methods depending on the student's interests).

Project

The project consists of implementing and benchmarking appropriate methods for regression/prediction of mass transport properties. The project will give you opportunities to investigate e. g. single-channel and multi-channel 2D CNNs, data augmentation schemes, and hyperparameter optimization. You should have an interest in machine learning but good knowledge in statistics, spatial statistics, and physics is beneficial to understand the underlying problem and its relevance. Knowledge of a major deep learning library (preferably TensorFlow/Keras, but it's up to you) is very beneficial.

References

Prifling et al, 2021, to appear online soon, available on request
Röding et al, 2020, https://www.nature.com/articles/s41598-020-72085-5

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