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Machine learning prediction of Lennard-Jones fluid self-diffusion in pores

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Porous materials are widely used in industrial applications (e.g., catalysis and separations) and diffusion of liquids within these materials can often control performance. Self-diffusion coefficients are typically obtained from molecular dynamics (MD) simulations in which the forces and trajectories of particles are calculated via Newtonian physics for millions of time steps. While MD provides accurate diffusion coefficients and can be tailored to a variety of circumstances (e.g., diffusion in pores), it is computationally expensive and requires large systematic studies in order provide insight as to which molecular properties affect diffusion. To provide a quicker, more computationally efficient alternative, we trained a variety of machine learning algorithms from simple linear models to complex convolutional neural networks to predict the diffusion of Lennard-Jones particles in a variety of ideal pore shapes. During the feature selection process, extra consideration was given to select features that are easy to obtain and understand by non-experts. Not only can these machine learning algorithms accurately predict diffusion coefficients at a fraction of the computational cost of MD, but they provide the opportunity to study the important features that contribute to the diffusion coefficient values. Insights obtained from studying the feature importance of these models can provide further understanding to the diffusion in porous media and enhance the materials design process for future porous materials used in industrial processes.

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References

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