De Novo Discovery of Nanoporous Structures by Machine Learning

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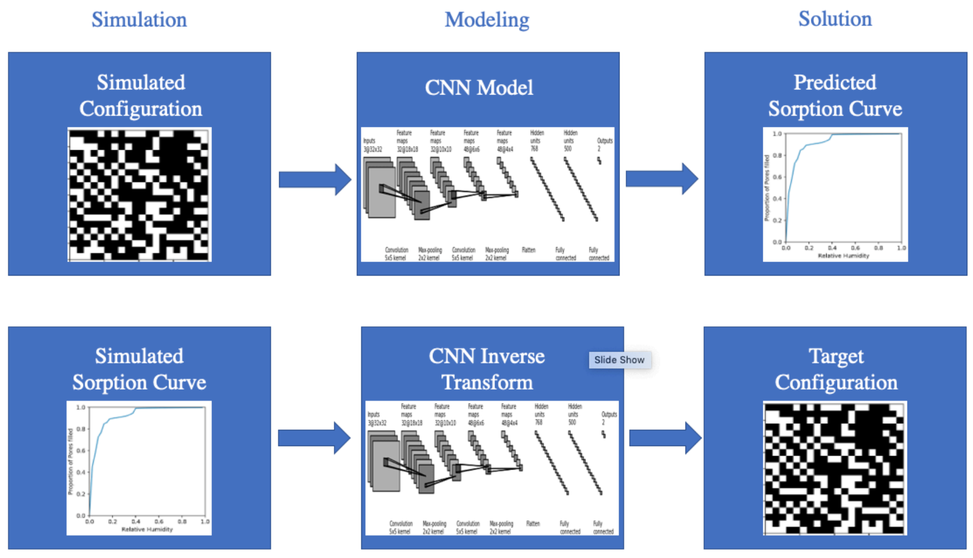
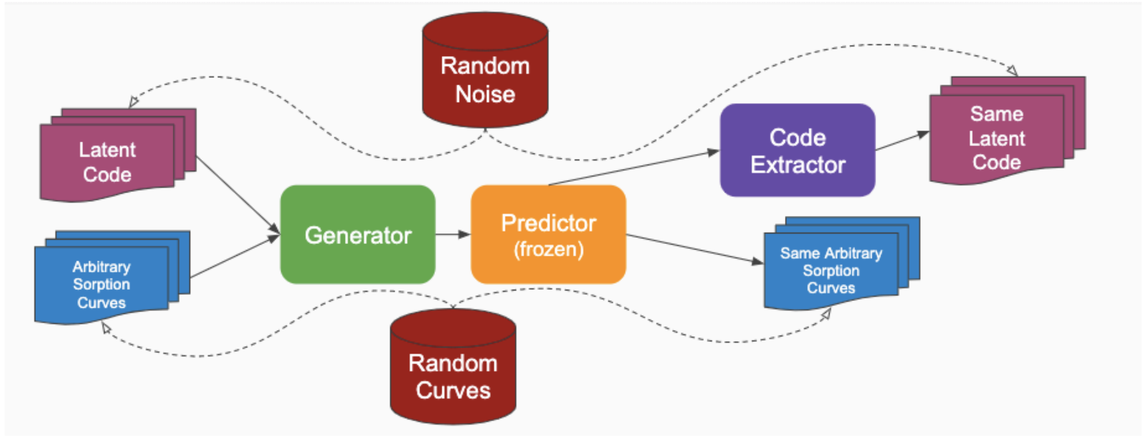
Motivation



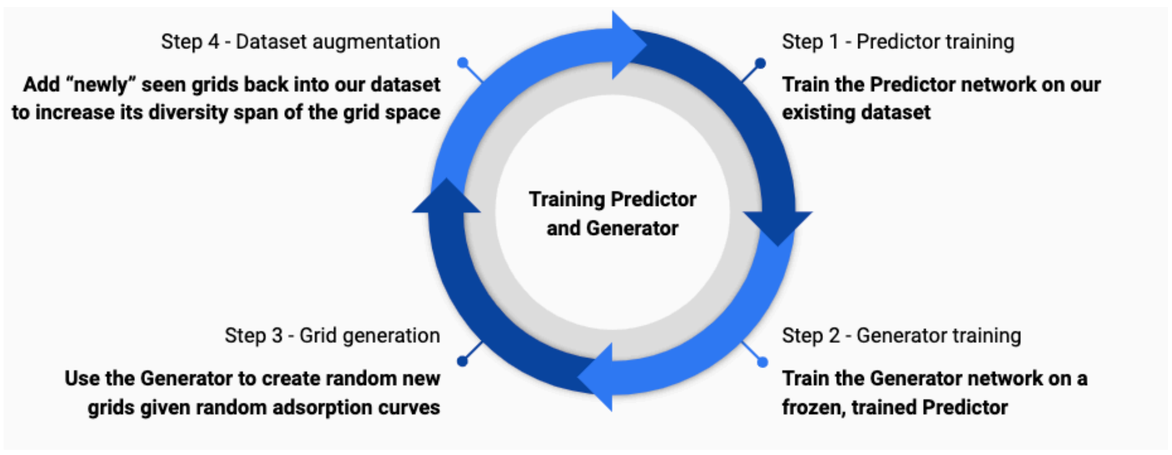
- Nanoporous materials have various technological applications, including gas separation, gas storage, catalytic transformations, …; the functionalities strongly depend on their pore size and shape distribution.
- Density functional theory (DFT) simulation is able to give a sorption curve with any given configuration, but it does not offer inverse transform.
- Can one model speed up the process of simulation and reveal the atomic structure of a material with a given sorption curve?

Methods



- We built one convolutional neural network(CNN) (as predictor) and another machine learning model (as generator) for simulation and inverse transform, respectively.
- System: 10^{117} configurations in a 20x20 grid considering all 400 translations, 4 reflections, and 4 rotations.
- Predictor: Grids -> Curves
- Generator: Curves x Latent Code -> Grids

Training Process



Activation Function:

- Unlike classic sigmoid function, binary sigmoid function will generate a binary value either 0 or 1 for each cell.
- To avoid larger errors when rounding numbers around 0.5.

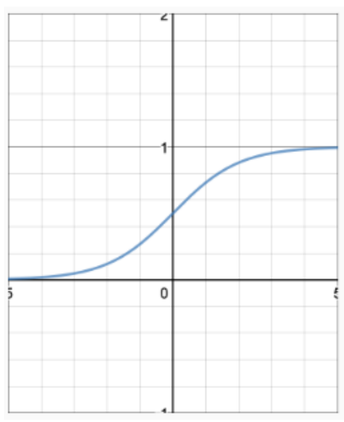


Fig. 1 Classic Sigmoid Function

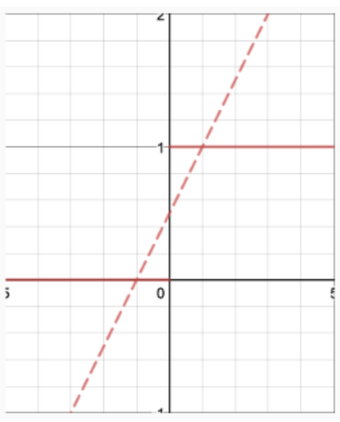


Fig. 2 Binary Sigmoid Function

Latent Code:

- There are several grid configurations mapping to one adsorption curve. Therefore, it is an one-to-many relationship to convert a curve back to a grid subspace.
- Latent code identifies each grid subspace if there exists some simple mapping from latent codes to grid subspace.

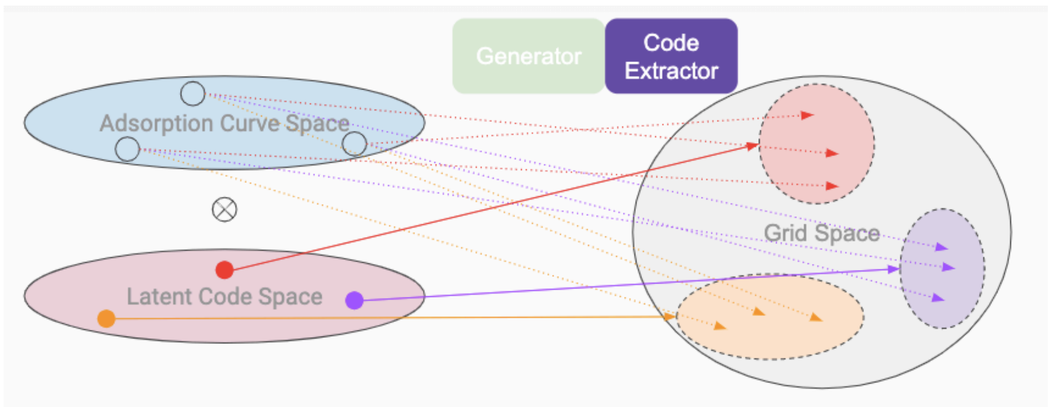


Fig. 3 Latent Code Augmentation Visualization

Results and Discussion

Predictor:

- Predictor yields a differentiable curve that is in excellent agreement with DFT simulation.
- The level of agreement is comparable with the target curve.
- Predictor simulates DFT simulations and performs faster computations.

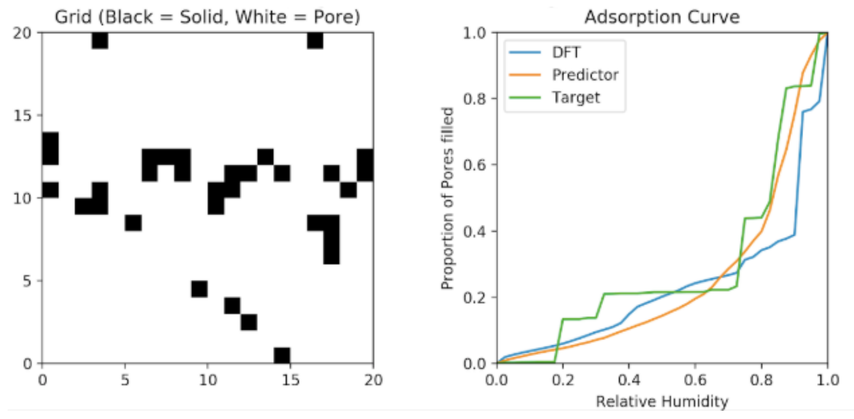


Fig. 4 DFT Simulation and Predictor vs. Target Curve

Generator:

- Generator is a deconvolutional neural network trained on inverting the predictor network.
- Generator makes a simulation of the behavior of predictor

Fine-Grained Optimization:

- Alternative optimization strategies, like swarm and steepest descent, are used for better precision after generator.

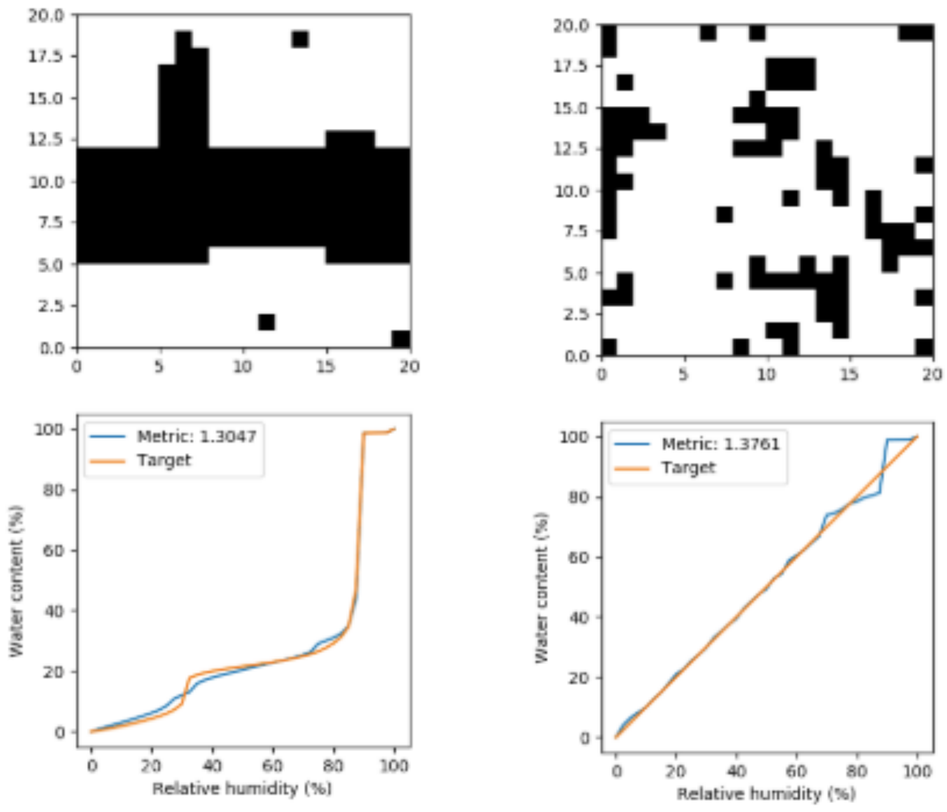


Fig. 5 Particle Swarm Optimization

Fig. 6 Steepest Descent

Conclusions

- CNN is able to capture the mutual relationship between atomic configurations and adsorption curves precisely.
- CNN is fairly inversible even though it is not designed to be inversible, which suggests that it is possible to invert networks through some mean other than designing its structure to be a certain shape.
- That inverting a CNN is possible through just correct training parameters and it might not be heavily dependent on the structure

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