Latent Variable Gaussian Processes and Bayesian Optimization Implementation to Determine Top-performing Metal-organic Frameworks

Research Objective

Metal-organic Frameworks (MOFs) are a class of nanoporous crystalline materials that are highly versatile and have a broad range of applications. Experimental synthesis cannot comprehensively explore the MOF-space, while common computation approaches such as high-throughput screening are computationally expensive. Our objective is to implement a novel computational method, Latent Variable Gaussian process (LVGP) and Bayesian optimization (BO), to study the MOF-space. This new approach is aimed to significantly reduce the computational cost by limiting the number of molecular simulations, while ensuring that top-performing MOFs are determined.

Metal-Organic Frameworks

Methodologies

Combined workflow of molecular simulations and LVGP-BO implemented in this work

Results

- Successfully implemented LVGP-BO to determine top-performing MOFs
- Automated the process to find potential MOFs with different topologies and different single objective functions

Discussion

- For a physical model with qualitative variables, a quantitative 2-D Latent Variable representation can explain the underlying effects on the property
- By only scanning less than 5% of the 40,500 sample dataset, LVGP-BO identified more than 80% of Top 25 best performing MOFs for CO₂ Working Capacity and N₂ / CO₂ Selectivity properties.

Conclusions

References