The Summer Undergraduate Research Fellowship (SURF) Symposium
3 August 2017
Purdue University, West Lafayette, Indiana, USA

Applying Machine Learning to Computational Chemistry: Can We Predict Molecular Properties Faster without Compromising Accuracy?

Hanjing Xu
Department of Computer Science, Purdue University
Pradeep K. Gurunathan, and Lyudmila V. Slipchenko
Department of Chemistry, Purdue University

ABSTRACT

Non-covalent interactions are crucial in analyzing protein folding and structure, function of DNA and RNA, structures of molecular crystals and aggregates, and many other processes in the fields of biology and chemistry. However, it is time and resource consuming to calculate such interactions using quantum-mechanical formulations. Our group has proposed previously that the effective fragment potential (EFP) method could serve as an efficient alternative to solve this problem. However, one of the computational bottlenecks of the EFP method is obtaining parameters for each molecule/fragment in the system, before the actual EFP simulations can be carried out. Here we present a neural network model that is trained by pre-calculated EFP parameters for a set of fragment geometries, to predict the multipole moment parameters for the fragments with arbitrary geometries. We perform Monte Carlo simulation to assess accuracy of the model. The results demonstrate the ability to predict multipole moments within acceptable margin of error given that the training set is closely spaced. These results contribute towards extending the applicability of the EFP method to new types of chemistries and improving the accuracy and computational efficiency of describing non-covalent interactions.

KEYWORDS

Non-covalent interaction simulations, EFP method, machine learning