Xufeng Cai
xufengcai.com
Email : zephyr@sjtu.edu.cn
+86-187-2165-9721

Research Experience

Gradient-free Consensus-based Global Optimization Methods Shanghai, China
Institute of Natural Sciences, SJTU; Advised by Prof. Shi Jin and Prof. Xiaoqun Zhang *Sept. 2019 – Present*

- Studied the convergence of the consensus-based global optimization method from the aspect of stochastic analysis.
- Implemented relevant algorithms to solve the logistic regression and compressive sensing problems with l_0 regularization. Currently conducting further numerical experiments on optimization problems in deep learning.
- Developing a relevant theoretically principled hybrid gradient method to improve the numerical performance and widen the gamut of practical use.

Deep Generative Model for Molecular Graphs Urbana-Champaign, IL, USA
Department of Computer Science, UIUC; Advised by Prof. Jian Peng *July 2019 – Sept. 2019*

- Implemented the sequential generative model for molecular graphs (DGMG) proposed by DeepMind, using RDKit Cheminformatics toolkit and DGL python library by AWS Amazon.
- Deployed the batch-training and parallel-training logics to accelerate the auto-regressive generative model training.
- Improved the performance of the original DGMG model by designing an innovative generating process with node degree constraints and replacing atoms with chemical radical groups as generating tokens.
- Tested our generative model on the Molecular Sets Benchmarking Platform, and achieved high performance in similarity metrics comparable to recent SOTA algorithms with fewer parameters and more malleable architectures.

Application of Deep Learning in Molecular Dynamics Shanghai, China
Institute of Natural Sciences, SJTU; Advised by Prof. Jinglai Li and Prof. Liang Hong *May 2018 – June 2019*

- Processed raw data collected from molecular dynamics (MD) data simulated with LAMMPS for deep neural network (DNN) modeling, using Python and the DeePMD toolkit.
- Designed and evaluated deep neural network architectures to predict force fields with processed data.
- Improved the current model by adopting active learning to interactively explore the conformation space.

Application of Machine Learning in the Analysis of Alloy Phase Transition Shanghai, China
Department of Computer Science and Engineering, SJTU; Advised by Prof. Xiaotie Deng *May 2017 – Oct. 2017*

- Extracted features and labels from the raw data of alloy phase transition according to the knowledge of material science. Organized them into the form of DataFrame in Pandas to apply statistical learning models.
- Trained and validated machine learning regression models such as GBDT and RandomForest. Applied cross validation to optimize models, and most prediction accuracies reached above 80% to 90%.
- Wrote reports that explained the prediction methodology.