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Research Experience

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

- Studied the convergence of the consensus-based global optimization method from the aspect of stochastic differential equations.
- Implemented the theoretical algorithm to solve the logistic regression and compressing sensing problems with l_0 regularization.
- Will develop a hybrid gradient method based on the consensus-based global optimization method to improve the numerical performance.

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

- Implemented the original sequential generative model for molecular graphs (DGMG) proposed by DeepMind, using RDKit Cheminformatics toolkit and DGL python library by AWS Amazon.
- Developed the batched-training version and parallel-training version on CPUs to accelerate the model.
- Improved the performance of the original DGMG model by innovating the generating process with ideas of 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 comparable to recent SOTA algorithms in similarity metrics.

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

- Applied LAMMPS to generate raw data from molecular dynamics simulation and processed raw data with Python.
- Designed deep neural networks to predict force fields with the processed raw data using DeePMD toolkit.
- Evaluated the prediction of the network by running MD for larger systems and longer time periods. Tried to improve the current model by implementing more efficient Fast Monte Carlo Methods and additional features.

Application of Machine Learning in the Analysis of Alloy Phase Transition Shanghai, China
Department of Computer Science and Engineering at 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 to apply models by using Pandas in Python.
- 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.