Xufeng Cai

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EDUCATION

Shanghai Jiao Tong University

Shanghai, China Sept. 2016 - Present

B.S. in Mathematics

• Overall GPA: 3.64/4.30 (86.1/100)

- Selected to Zhiyuan Honors Program, an elite program for students in the top 5%
- Research Intern in the Department of Computer Science in University of Illinois, Urbana-Champaign
- Selective Awards: Outstanding Winner in the Interdisciplinary Contest in Modeling (top 0.16% in over 20,000 teams), Merit Student (top 6% in school, awarded to those with comprehensive development)
- Selective Course Grades: C++ Programming: 95, Computational Methods for Multi-scale Physical Problems: 95, Functional Analysis: 95, Algebraic Number Theory: 93, Abstract Algebra: 91, Partial Differential Equations: 90

Hertford College, University of Oxford

Oxford, UK

Exchange Student in Math and Physics Program

June 2018 - July 2018

• Final Grade: A (Manifolds and Group Theory)

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.

Adaptive Moving Mesh Method for Blow-up Equations with e^{μ} Nonlinearity Shanghai, China Apr. 2019 - June 2019 Coursework for "Numerical Methods for Ordinary and Partial Differential Equations" at SJTU

- Studied relevant papers and books to address the blow-up phenomenon of equations with e^{μ} nonlinearity.
- Implemented the adaptive moving mesh method to solve the blow-up equation and reduce the numerical error compared with the results of fixed uniform mesh.
- Wrote reports to present the theoretical analysis and numerical results for e^{μ} -nonlinear equations.

Climate-based Fragility Measurement Model for Regions in the World

• Designed an index SPEC to evaluate regional fragility concerning effects of climate change.

Shanghai, China Feb. 2018

- The Interdisciplinary Contest in Modeling, Comap
- Collected and cleaned relevant data of 178 countries worldwide to test our model. Our SPEC score corresponded to the traditional Fragile State Index but stressed the effects of climate change.
- Wrote reports to present our model and analysis of simulation results. Our team was designated as Outstanding Winner (top 0.16% in over 20,000 teams in the world).

Extracurricular Activities

Class Assistant of Mathematics Class, Grade 2017 of Zhiyuan College

Shanghai, China

Zhiyuan College, Shanghai Jiao Tong University

Sept. 2017 - Present

• Tutor students in various aspects, including academic study, daily life management, etc.

International Youth Leadership Finance Summit, SAIF

Shanghai, China

Participant representing Shanghai Jiao Tong University

Jan. 2019

- Designed AI solutions for a real health company to its in vitro diagnostics and pharmaceutical business.
- Presented a roadshow to the investors in order to seek equity financing.

AWARDS & SCHOLARSHIPS

- Outstanding Winner | The Interdisciplinary Contest in Modeling, Comap (top 0.16% in over 20,000 teams) 2018
- Xingcai Scholarship | Shanghai Jiao Tong University (0.01% in Zhiyuan College)

2018 2018

Merit Student | Shanghai Jiao Tong University (6% in school)

- 2017 & 2018 & 2019
- Academic Excellence Scholarship | Shanghai Jiao Tong University (top 10% in school)
- Merit Scholarship of Zhiyuan Honors Program | Shanghai Jiao Tong University 2016 & 2017 & 2018 & 2019
- Kaiyuan Encouragement Scholarship | Shanghai Jiao Tong University (0.05% in Zhiyuan College)

2017

SKIILS

- Technical: C++, Python, Matlab, R, SQL, HTML, LATEX
- Language: English (TOEFL 105; GRE V:152, Q:170, AWA:4)