

Zhongkai HAO

Personal Information

Phone: 18800130159
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Date of Birth: 3 October, 2001
Nationality: Chinese
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Experience

PRESENT | Ph.D student at Department of Electronic Engineering, Tsinghua University

Education

SEPT 2021 - PRESENT | **PhD student in Electronic Engineering, Tsinghua University**
Supervisor: Jun Zhu and Jian Song

SEPT 2017 - JUNE 2021 | **Bachelor Degree in Mathematics, University of Science and Technology of China (USTC)**
Major: Information and Computation Science | RANKING: 2/54

Awards

AUTUMN 2022 | Qiangwei Xinhe Scholarship
AUTUMN 2020 | Yang Yuanqing Scholarship
AUTUMN 2018 | National Scholarship (5%)
AUTUMN 2019 | Merit student award
AUTUMN 2017 | Outstanding Freshmen's Scholarship, Golden Prize

Research Interest

- Physics-Informed Machine Learning for Science and Engineering
- Robust Machine Learning for Computer Vision
- Graph Neural Networks: theory and applications on chemical data
- Learning with Limited Data: unsupervised learning and active learning

Computer Skills

- **Programming Languages:** Matlab, Python Pytorch/Tensorflow, C/C++
- **Softwares:** L^AT_EX, Microsoft Office, Labview, Mathematica, COMSOL

Publications

- **Physics-Informed Machine Learning: A Survey on Problems, Methods and Applications.**
Zhongkai Hao, Songming Liu, Yichi Zhang, Chengyang Ying, Yao Feng, Hang Su, Jun Zhu
arxiv, e-print
- **Full-Atom Protein Pocket Design via Iterative Refinement.**

Zaixi Zhang, Zepu Lu, **Zhongkai Hao**, Marinka Zitnik, Qi Liu

Thirty-seventh Conference on Neural Information Processing Systems (NeurIPS), New Orleans, USA, 2023 (**Spotlight**)

- **GNOT: A General Neural Operator Transformer for Operator Learning.**
Zhongkai Hao, Chengyang Ying, Zhengyi Wang, Hang Su, Yinpeng Dong, Songming Liu, Ze Cheng, Jun Zhu, Jian Song
International Conference on Machine Learning (ICML), Hawaii, USA, 2023
- **NUNO: A General Framework for Learning Parametric PDEs with Non-Uniform Data.**
Songming Liu, **Zhongkai Hao**, Chengyang Ying, Hang Su, Ze Cheng, Jun Zhu
International Conference on Machine Learning (ICML), Hawaii, USA, 2023
- **MultiAdam: Parameter-wise Scale-invariant Optimizer for Multiscale Training of Physics-informed Neural Networks.**
Jiachen Yao, Chang Su, **Zhongkai Hao**, Songming Liu, Hang Su, Jun Zhu
International Conference on Machine Learning (ICML), Hawaii, USA, 2023
- **Bi-level Physics-Informed Neural Networks for PDE Constrained Optimization using Broyden's Hypergradients.**
Zhongkai Hao, Chengyang Ying, Hang Su, Jun Zhu, Jian Song, Ze Cheng
The Eleventh International Conference on Learning Representations (**ICLR**), Kigali Rwanda, 2023
- **Equivariant Energy-Guided SDE for Inverse Molecular Design.**
Fan Bao, Min Zhao, **Zhongkai Hao**, Peiyao Li, Chongxuan Li, Jun Zhu
The Eleventh International Conference on Learning Representations (**ICLR**), Kigali Rwanda, 2023
- **A Unified Hard-Constraint Framework for Solving Geometrically Complex PDEs.**
Songming Liu, **Zhongkai Hao**, Chengyang Ying, Hang Su, Jun Zhu, Ze Cheng
Thirty-sixth Conference on Neural Information Processing Systems (NeurIPS), New Orleans, 2022
- **GSmooth: Certified Robustness against Semantic Transformations via Generalized Randomized Smoothing.**
Zhongkai Hao, Chengyang Ying, Yinpeng Dong, Hang Su, Jian Song, Jun Zhu
International Conference on Machine Learning (**ICML**), Baltimore, USA, 2022 (CCF-A Conference).
- **Cluster Attack: Query-based Adversarial Attacks on Graphs with Graph-Dependent Priors.**
Zhengyi Wang, **Zhongkai Hao**, Ziqiao Wang, Hang Su and Jun Zhu
International Joint Conference on Artificial Intelligence (**IJCAI**), Online, 2022 (**Long Oral**, CCF-A Conference)
- **An Active Semi-supervised Graph Neural Network for Molecular Property Prediction.**
Zhongkai Hao, Chengqiang Lu, Zhenya Huang, Hao Wang, Qi Liu, Zheyuan Hu, Cheekong-Lee, Enhong Chen
Special Interest Group on Knowledge Discovery and Data Mining (**SIGKDD' 2020**) (CCF-A Conference)
- **A two-stage 3D CNN based learning method for spontaneous micro-expression recognition.**
Sirui Zhao, Hanqing Tao, Yangsong Zhang, Tong Xu, Kun Zhang, **Zhongkai Hao**, Enhong Chen
Neurocomputing, 276-289, 448, Elsevier

Professional Services

Reviewer for:

- IJCAI 2023, ICML 2023, NeurIPS 2023, ICLR 2024
- NeurIPS 2022, ICML 2022,
- Adversarial Machine Learning Workshop, ICML 2021,
- SIGKDD 2020.

Teaching

- 2023 Spring, TA in Statistical Machine Learning, instructed by Prof Hang Su.

- 2022 Spring, TA in Statistical Machine Learning, instructed by Prof Hang Su.

Activities

SPRING, 2021	The 7-th place in SIGKDD Cup 2020 Graph adversarial attack and defense challenge.
AUTUMN, 2018	Course Work of Differential Equations, USTC A numerical simulation program for lightening.
SUMMER 2018	A PID based wavelength control system, USTC Using Proportional–Integral–Derivative method to control the wavelength of a laser and automatic tuning of PID parameters.
AUTUMN. 2017	Big Data & Mathematical Modeling Contest, <i>Third Prize</i>, USTC Finding solutions of a multiple salesman like problem (MTSP) with time window using improved genetic algorithm.