

Xitong Zhang

RESEARCH INTERESTS

- Learning on Graphs
- AI for Science
- Generalization in Machine Learning

EDUCATION

- **Michigan State University** Michigan, USA
Doctorate degree in Computational Mathematics, Science and Engineering May 2018 - present
Master's degree in Computer Science and Engineering
- **Worcester Polytechnic Institute** Massachusetts, USA
Master's degree in Computer Science August 2016 - May 2018
- **Hunan University** Hunan, China
Bachelor's degree in Intelligence Science and Technology September 2012 - June 2016

INTERNSHIPS

- **Qualcomm Technologies, Inc.** California, USA
Machine Learning Engineer May 2023 - August 2023
- **Los Alamos National Laboratory, Applied Mathematics and Plasma Physics** New Mexico, USA
Graduate Research Assistant March 2022 - Aug 2022
- **Los Alamos National Laboratory, Geophysics** New Mexico, USA
Graduate Research Assistant June 2021 - Aug 2021
- **Los Alamos National Laboratory, Geophysics** New Mexico, USA
Graduate Research Assistant May 2020 - Aug 2020

OPEN SOURCE PROJECTS

- **PyTorch Geometric Signed Directed** [[Link](#)]
PyTorch Geometric Signed Directed consists of various signed and directed geometric deep learning, embedding, and clustering methods from a variety of published research papers and selected preprints.
- **OpenFWI** [[Link](#)]
OpenFWI is the first large-scale open-access multi-structural seismic imaging dataset for machine learning-driven Full Waveform Inversion. It includes twelve datasets synthesized from different priors, including one 3D dataset, and also provides baseline experimental results with four deep-learning methods.

FELLOWSHIPS & SCHOLARSHIPS

- CNLS Fellowship Los Alamos National Laboratory, 2021
- Applied Machine Learning Summer Research Fellowship Los Alamos National Laboratory, 2020
- Graduate Office Fellowship Michigan State University, 2022
- Graduate Office Fellowship Michigan State University, 2020
- The First Prize Scholarship Hunan University, 2014
- The Second Prize Scholarship Hunan University, 2014
- Heyuan Special Scholarship Hunan University, 2014

PUBLICATIONS

* indicates equal contribution

Generalization in Machine Learning

1. “Unlocking Tuning-Free Generalization: Minimizing the PAC-Bayes Bound with Trainable Priors.”
Xitong Zhang, Avrajit Ghosh, Guangliang Liu, and Rongrong Wang (under review)
2. “PAC-tuning: Fine-tuning Pre-trained Language Models with PAC-driven Perturbed Gradient Descent.”
Guangliang Liu, Zhiyu Xue, **Xitong Zhang**, Kristen Johnson, Rongrong Wang (**EMNLP**, 2023)
3. “Implicit regularization in Heavy-ball momentum accelerated stochastic gradient descent.”
Avrajit Ghosh*, He Lyu*, **Xitong Zhang**, and Rongrong Wang
International Conference on Learning Representations (**ICLR**), 2023
Spotlight (5.6% \approx 280/4956)

Learning on Graphs

1. “PyTorch Geometric Signed Directed: A Software Package on Graph Neural Networks for Signed and Directed Graphs.”
Yixuan He, **Xitong Zhang**, Junjie Huang, Benedek Rozemberczki, Mihai Cucuringu, and Gesine Reinert (under review)
2. “Can Directed Graph Neural Networks be Adversarially Robust?”
Zhichao Hou, **Xitong Zhang**, Wei Wang, Charu C Aggarwal, Xiaorui Liu (under review)
3. “Spatiotemporal graph convolutional networks for earthquake source characterization.”
Xitong Zhang*, Will Reichard-Flynn*, Miao Zhang, Matthew Hirn, and Youzuo Lin
Journal of Geophysical Research (**JGR**): Solid Earth, 127(11), 2022
4. “Magnet: A neural network for directed graphs.”
Xitong Zhang, Yixuan He, Nathan Brugnone, Michael Perlmutter, and Matthew Hirn
Advances in neural information processing systems (**NeurIPS**), 2021
5. “Shoreline: Data-Driven Threshold Estimation of Online Reserves of Cryptocurrency Trading Platforms.”
Xitong Zhang, He Zhu, and Jiayu Zhou
Association for the Advancement of Artificial Intelligence (**AAAI**), 2020
Oral (5.7% \approx 438/7737)
6. “Boosted Trajectory Calibration for Traffic State Estimation.”
Xitong Zhang, Liyang Xie, Zheng Wang, and Jiayu Zhou
IEEE International Conference on Data Mining, (**ICDM**), 2019
Long paper, (9.1% \approx 95/1046)

AI for Science

1. “Enhanced prediction accuracy with uncertainty quantification in monitoring CO2 sequestration using convolutional neural networks.”
Yanhua Liu, **Xitong Zhang**, Ilya Tsvankin, Youzuo Lin (under review)

2. “Unsupervised Learning of Full-Waveform Inversion: Connecting CNN and Partial Differential Equation in a Loop.”
Peng Jin*, **Xitong Zhang***, Yinpeng Chen, Sharon X Huang, Zicheng Liu, and Youzuo Lin
International Conference on Learning Representations (**ICLR**), 2022
3. “Making Invisible Visible: Data-Driven Seismic Inversion With Spatio-temporally Constrained Data Augmentation.”
Yuxin Yang, **Xitong Zhang**, Qiang Guan, and Youzuo Lin
IEEE Transactions on Geoscience and Remote Sensing (**TGRS**) 2022.
4. “Extremely weak supervision inversion of multiphysical properties.”
Shihang Feng, Peng Jin, **Xitong Zhang**, Yinpeng Chen, David Alumbaugh, Michael Commer, and Youzuo Lin
Second International Meeting for Applied Geoscience & Energy, 2022
5. “Enhancing data-driven seismic inversion using physics-guided spatiotemporal data augmentation.”
Yuxin Yang, **Xitong Zhang**, Qiang Guan, and Youzuo Lin
SEG/AAPG/SEPM First International Meeting for Applied Geoscience & Energy, 2021
6. “Connect the Dots: In Situ 4-D Seismic Monitoring of CO₂ Storage With Spatio-Temporal CNNs.”
Shihang Feng, **Xitong Zhang**, Brendt Wohlberg, Neill P. Symons, and Youzuo Lin
IEEE Transactions on Geoscience and Remote Sensing (**TGRS**), 2021
7. “A deep learning-based segmentation pipeline for profiling cellular morphodynamics using multiple types of live cell microscopy.”
Junbong Jang, Chuangqi Wang, **Xitong Zhang**, Hee June Choi, Xiang Pan, Bolun Lin, Yudong Yu, Carly Whittle, Madison Ryan, Yenyu Chen, and Kwonmoo Lee
Cell reports methods, 2021

WORKSHOPS AND ABSTRACTS

1. “Supervised vs. unsupervised deep learning full waveform inversion: a case study at CCUS site, San Juan NM.”
Hanchen Wang, Shihang Feng, Youzuo Lin, Yinpeng Chen, **Xitong Zhang**, Peng Jin, Rajesh J Pawar, and George Drake Guthrie
The International Geoscience and Remote Sensing Symposium; 2023
2. “An Open-source Platform to Facilitate Data-driven FWI Research.”
Shihang Feng, Chengyuan Deng, Hanchen Wang, **Xitong Zhang**, Qili Zeng, Peng Jin, Yinan Feng, Youzuo Lin, Yinpeng Chen
AGU Fall Meeting Abstracts 2022
3. “Seismic Source Characterization using Physics-Guided Graph Convolutional Neural Network.”
Will Reichard-Flynn, **Xitong Zhang**, Miao Zhang, Youzuo Lin
AGU Fall Meeting Abstracts 2022
4. “Weakly Supervised Inversion of Multi-physics Data for Geophysical Properties.”
Shihang Feng, Peng Jin, Yinpeng Chen, **Xitong Zhang**, Zicheng Liu, David Alumbaugh, Michael Commer, and Youzuo Lin
2nd AI for Science Workshop, ICML 2022

5. “4D Seismic Monitoring and Forecasting of CO2 Sequestration with Neural Networks.”
Shihang Feng, **Xitong Zhang**, Brendt Wohlberg, Neill Symons, and Youzuo Lin
AGU Fall Meeting Abstracts, 2021
6. “Earthquake Source Characterization with Graphical Deep Learning.”
Xitong Zhang, Miao Zhang, and Youzuo Lin
AGU Fall Meeting Abstracts 2020
7. “How Good Is Your Scientific Data Generative Model?”
Yuxin Yang, Ben Gremillion, **Xitong Zhang**, Youzuo Lin, Brendt Wohlberg, Qiang Guan
IEEE/ACM Workshop on Artificial Intelligence and Machine Learning for Scientific Applications, 2020
8. “Shoreline: Data-Driven Threshold Estimation of Online Reserves of Cryptocurrency Trading Platforms (Student Abstract).”
Xitong Zhang, He Zhu, Jiayu Zhou
Proceedings of the AAAI Conference on Artificial Intelligence (**AAAI**), 2020

COMPETITION AWARDS

- Mathematical Contest in Modeling (MCM) Honorable Mention, 2016
- Mathematical Contest in Modeling (MCM) Honorable Mention, 2015
- The 9th Chinese Information Application Level Contest National Second Prize, 2014
- China Robot Competition and The RoboCup China Open First Prize, 2014

TEACHING & ADVISING

- Graduate Mentor of the Graduate Women in Science Mentoring Program Michigan State University, 2023
- Guest Mentor of Graduate Research Assistants Yunnan Normal University, 2023
- Guest Mentor of Graduate Research Assistants Los Alamos National Laboratory, 2021–2022
- Teaching Assistant of:
 - Introduction to Computational Modeling (CMSE 201) Michigan State University, 2021
Responsibilities:
 - * Conducted in-class coding sessions for all lectures.
 - * Hosted regular office hours for student consultations.
 - * Managed and executed grading procedures.
 - Machine Learning (CSE 847) Michigan State University, 2020
Responsibilities:
 - * Led review lectures to reinforce core concepts.
 - * Maintained regular office hours for student support.
 - * Carried out grading duties.
 - Large Scale Data Analysis for MSBA (CSE 891) Michigan State University, 2018
Responsibilities:
 - * Facilitated regular office hours for student queries.
 - * Carried out grading duties.

SEMINAR TALKS

- **Visiting Talk** Georgia Institute of Technology, USA, 2023
Unlocking Tuning-Free Generalization: Minimizing the PAC-Bayes Bound with Trainable Priors
- **Ph.D. Lecture Series** Qualcomm, USA, 2023
Explicit and Implicit Regularization in Machine Learning
- **Undergraduate Student Research Training Seminar** Yunnan Normal University, China, 2023
Introduction of Spatiotemporal Data Mining–Applications in Traffic and Geophysics
- **Center for Nonlinear Studies Seminar** Los Alamos National Laboratory, USA, 2021
Data-Driven Seismic Inversion–Learning to Solve Inverse Problems via Physics-Informed Networks

SERVICES

Conference reviewer:

- International Conference on Learning Representations (ICLR) 2024
- Neural Information Processing Systems (NeurIPS) 2022/2023
- Association for the Advancement of Artificial Intelligence (AAAI) 2023/2024
- Learning on Graphs Conference (LoG) 2023/2024
- Symposium on Applied Computational Intelligence and Informatics (SACI) 2023
- ACM SIGKDD Conference on Knowledge Discovery and Data Mining (KDD) 2020/2022
- International Meeting for Applied Geoscience & Energy (IMAGE) 2022

Journal reviewer:

- IEEE Transactions on Geoscience and Remote Sensing (ISSN: 1558-0644), 2023
- Biology (ISSN: 2079-7737), 2022
- Computation (ISSN 2079-3197), 2022
- Neurocomputing (ISSN: 0925-2312), 2018-2020

SKILLS

Python, Matlab, C/C++, HDF5, Keras, TensorFlow, PyTorch, Scikit-learn, OpenCV, Matplotlib, Seaborn, NumPy, SciPy, Pandas, OpenMP, MPI, D3.js, Slurm, Azure, AWS.