9500 Gilman Drive, Mail Code 0404 E-mail: roseyu@ucsd.edu

Department of Computer Science and Engineering

University of California, San Diego

Phone: (858) 246-4724

Office: CSE 4216

La Jolla, CA 92093-0404

Homepage: www.roseyu.com

RESEARCH Spatiotemporal Machine Learning, Deep Learning, AI for Science.

CURRENT University of California, San Diego, La Jolla, California

Appointment Associate Professor, Department of Computer Science and Engineering July 2024 - Present

Previous University of California, San Diego, La Jolla, California

APPOINTMENT Assistant Professor, Department of Computer Science and Engineering July 2020 - June 2024

Google Cloud, San Diego, California

Visiting Researcher, Cloud AI Research Oct 2021 - March 2023

Northeastern University, Boston, Massachusetts

Assistant Professor, Khoury College of Computer Sciences Aug 2018 - June 2020

Network Science Institute, College of Engineering, Physics (By Courtesy)

California Institute of Technology, Pasadena, California

Postdoctoral Scholar, Computing + Mathematical Sciences Aug 2017 - Aug 2018

• Advisors: Anima Anandkumar, Yisong Yue

Stanford University, Palo Alto, California

Visiting Researcher, Computer Science Department Aug 2016 - Oct 2016

• Host: Christopher Ré

IBM Research, Yorktown Heights, New York

Research Intern June 2015 - Aug 2015

Yahoo! Labs, Sunnyvale, California

Research Intern June 2014 - Aug 2014

Intel Lab, Santa Clara, California

Research Intern May 2013 - Aug 2013

Microsoft R&D, Minghang, Shanghai

Program Manager Intern

June 2011 - June 2012

EDUCATION University of Southern California, Los Angeles, California

Ph.D., Computer Science, Computer Science Department

Aug 2012 - Aug 2017

Thesis: Tensor Learning for Large-Scale Spatiotemporal Analysis

Finalist in William F. Ballhaus, Jr. Prize for Excellence in Graduate Engineering Research

• Thesis Committee: Yan Liu (chair), Cyrus Shahabi (co-chair), Mahdi Soltanolkotabi

Zhejiang University, Hangzhou, Zhejiang, PRC

B.S in Computer Science, Chu Kochen Honors College Aug 2008 - June 2012

• Advisor: Zhihua Zhang

SELECTED AWARDS Best Paper Award, ICML ML for Earth System Modeling Workshop, July 2024 AND HONORS

Young Faculty Award, DARPA, June 2024

Outstanding Datasets and Benchmarks Paper Award, NeurIPS, Dec 2023

Early Career Awards for Scientists and Engineers, Army Research Office, May 2023

Faculty Research Award, NEC Laboratories America, March 2023

NSF CAREER Award, National Science Foundation, June 2022

Hellman Fellow, Hellman Fellows Fund, May 2022

Outstanding Faculty Researcher Award, JPMorgan, July 2021

Facebook Data Science Research Awards, Facebook Research, June 2021

Google Cloud Research Innovators, Google Cloud, March 2021

AWS Machine Learning Research Awards, Amazon Science, Feb 2021

Best Paper Award, NeurIPS ML for Public Health Workshop, Dec 2020

Adobe Data Science Research Awards, Adobe Research, March 2020

Google Faculty Research Award, Google Research, Feb 2020

Best Dissertation Award, University of Southern California, 2018

Best Paper Award, NIPS Time Series Workshop, 2017

SIGKDD Scholarship, ACM 50th Celebration of the Turing Award, San Francisco, 2017

Rising Stars in EECS, 40 Awardees in North America, MIT, 2015

Annenberg Graduate Fellowship, University of Southern California, 2012

Selected in ACM Heidelberg Laureate Forum, University of Heidelberg, 2013

Microsoft 2011 Young Fellowship, Microsoft Research Asia, 2011

International Forum (iF) Design Hanover Global Concept Award, iF, 2010

First prize in Undergraduate Research and Innovation, Zhejiang University, 2010

### Conference Publications

- [C1] Sumanth Varambally, Yian Ma, Rose Yu. "Discovering Mixtures of Structural Causal Models from Time Series Data." To Appear In *International Conference on Machine Learning* (ICML), 2024
- [C2] Jianke Yang, Nima Dehmamy, Robin Walters, Rose Yu. "Latent Space Symmetry Discovery."
  To Appear In International Conference on Machine Learning (ICML), 2024
- [C3] Ruijia Niu, Dongxia Wu, Kai Kim, Duncan Watson-Parris, Yian Ma, Rose Yu. "Multi-Fidelity Residual Neural Processes for Scalable Surrogate Modeling." To Appear In International Conference on Machine Learning (ICML), 2024

- [C4] Tao Wang, Bo Zhao, Sicun Gao, Rose Yu. "Understanding the Difficulty of Solving Cauchy Problems with PINNs." To Appear In Learning for Dynamics & Control Conference (L4DC), 2024
- [C5] Sophia Sun, Wenyuan Chen, Zihao Zhou, Sonia Fereidooni, Elise Jortberg, Rose Yu. "Data-Driven Simulator for Mechanical Circulatory Support with Domain Adversarial Neural Process." To Appear In Learning for Dynamics & Control Conference (L4DC), 2024
- [C6] Dongxia Wu, Tsuyoshi Idé, Aurélie Lozano, Georgios Kollias, Jiří Navrátil, Naoki Abe, Yian Ma, Rose Yu. "Learning Granger Causality from Instance-wise Self-attentive Hawkes Processes." In International Conference on Artificial Intelligence and Statistics (AISTATS), 2024
- [C7] Cai Zhou, Rose Yu, Yusu Wang. "On the Theoretical Expressive Power and Design Space of High Order Graph Transformers." In *International Conference on Artificial Intelligence and Statistics* (AISTATS), 2024
- [C8] Sophia Sun, Rose Yu. "Copula Conformal Prediction for Multi-step Time Series Forecasting." To Appear In *International Conference on Learning Representations* (ICLR), 2024
- [C9] Bo Zhao, Robert M. Gower, Robin Walters, Rose Yu. "Improving Convergence and Generalization Using Parameter Symmetries." To Appear In *International Conference on Learning Representations* (ICLR), 2024 Oral
- [C10] Zihao Zhou, Rose Yu. "Automatic Integration for Spatiotemporal Neural Point Processes". In Advances in Neural Information Processing Systems (NeurIPS), 2023
- [C11] Salva Rühling Cachay, Bo Zhao, Hailey James, Rose Yu. "DYffusion: A Dynamics-informed Diffusion Model for Spatiotemporal Forecasting". In Advances in Neural Information Processing Systems (NeurIPS), 2023
- [C12] Sungduk Yu, et al. "ClimSim: An open large-scale dataset for training high-resolution physics emulators in hybrid multi-scale climate models" In *Advances in Neural Information Processing Systems* (NeurIPS) Datasets and Benchmarks, 2023 **Best Paper**
- [C13] Dongxia Wu, Ruijia Niu, Matteo Chinazzi, Alessandro Vespignani, Yi-An Ma, Rose Yu. "Deep Bayesian Active Learning for Accelerating Stochastic Simulation". In *ACM SIGKDD Conference on Knowledge Discovery and Data Mining* (KDD), 2023
- [C14] Jianke Yang, Robin Walters, Nima Dehmamy, Rose Yu. "Generative Adversarial Symmetry Discovery". In *International Conference on Machine Learning* (ICML), 2023
- [C15] Dongxia Wu, Ruijia Niu, Matteo Chinazzi, Yi-An Ma, Rose Yu. "Disentangled Multi-Fidelity Deep Bayesian Active Learning" In *International Conference on Machine Learning* (ICML), 2023
- [C16] Chen Cai, Truong Son Hy, Rose Yu, Yusu Wang. "On the Connection Between MPNN and Graph Transformer". In *International Conference on Machine Learning* (ICML), 2023
- [C17] Zihao Zhou, Rose Yu. "Automatic Integration for Fast and Interpretable Neural Point Processes" In Annual Conference on Learning for Dynamics and Control(L4DC), 2023
- [C18] Sophia Sun, Robin Walters, Jinxi Li, <u>Rose Yu</u>. "Probabilistic Symmetry for Multi-Agent Dynamics". In *Annual Conference on Learning for Dynamics and Control* (L4DC), 2023
- [C19] Rui Wang, Yihe Dong, Sercan Ö. Arik, Rose Yu. "Koopman Neural Forecaster for Time Series with Temporal Distribution Shifts." In International Conference on Learning Representations (ICLR), 2023
- [C20] Bo Zhao, Iordan Ganev, Robin Walters, <u>Rose Yu</u>, Nima Dehmamy." Symmetries, flat minima, and the conserved quantities of gradient flow." In *International Conference on Learning Representations* (ICLR), 2023
- [C21] Bo Zhao, Nima Dehmamy, Robin Walters, Rose Yu "Symmetry Teleportation for Accelerated Optimization." In Advances in Neural Information Processing Systems (NeurIPS), 2022

- [C22] Rui Wang, Robin Walters, Rose Yu "Meta-Learning Dynamics Forecasting Using Task Inference." In Advances in Neural Information Processing Systems (NeurIPS), 2022
- [C23] Dongxia Wu, Matteo Chinazzi, Alessandro Vespignani, Yi-An Ma, Rose Yu Multi-fidelity Hierarchical Neural Processes. In Proceedings of ACM SIGKDD Conference on Knowledge Discovery and Data Mining (KDD), 2022
- [C24] Rui Wang, Robin Walters, Rose Yu "Approximately Equivariant Networks for Imperfectly Symmetric Dynamics" In *International Conference on Machine Learning* (ICML), 2022
- [C25] Peter Eckmann, Kunyang Sun, Bo Zhao, Mudong Feng, Michael Gilson, Rose Yu "LIMO: Latent Inceptionism for Targeted Molecule Generation" In Proceedings of International Conference on Machine Learning (ICML), 2022
- [C26] Zihao Zhou, Xingyi Yang, Ryan Rossi, Handong Zhao, Rose Yu. "Neural Point Process for Learning Spatiotemporal Event Dynamics" In Proceedings of Annual Conference on Learning for Dynamics and Control (L4DC), 2022
- [C27] Alan Li, Zihao Zhou, Elise Jortbeg, <u>Rose Yu</u>. "Generalization of Deep Sequence Models for Forecasting Aortic Pressure Cross-Cohort" In *Computing in Cardiology* (CinC), 2022.
- [C28] Alejandro Rodriguez Pascual, Ishan Mehta, Muhammad Khan, Frank Rodriz, Rose Yu. "Understanding why shooters shoot An AI-powered engine for basketball performance profiling" MIT Sloan Sports Analytics Conference (SSAC), 2022
- [C29] Nima Dehmamy, Robin Walters, Yanchen Liu, Dashun Wang, Rose Yu. "Automatic Symmetry Discovery with Lie Algebra Convolutional Network" In Proceedings of Advances in Neural Information Processing Systems (NeurIPS), 2021
- [C30] Dongxia Wu, Liyao Gao, Xinyue Xiong, Matteo Chinazzi, Alessandro Vespignani, Yi-An Ma, Rose Yu. "Quantifying Uncertainty in Deep Spatiotemporal Forecasting" In Proceedings of ACM SIGKDD Conference on Knowledge Discovery and Data Mining (KDD), 2021
- [C31] Rui Wang, Danielle Maddix, Christos Faloutsos, Yuyang Wang, Rose Yu. "Bridging Physics-based and Data-driven modeling for Learning Dynamical Systems", In Proceeding of Annual Conference on Learning for Dynamics and Control (L4DC), 2021
- [C32] Steven Wong, Lejun Jiang, Robin Walters, Tamás G. Molnár, Gábor Orosz, Rose Yu. "Physics-Guided Deep Learning for Traffic Forecasting using Vehicle-to-Vehicle Communication" In Proceeding of Annual Conference on Learning for Dynamics and Control (L4DC), 2021
- [C33] Robin Walters, Jinxi (Leo) Li, <u>Rose Yu</u>. "Trajectory Prediction using Equivariant Continuous Convolution", In *International Conference on Learning Representations* (ICLR), 2021
- [C34] Rui Wang, Robin Walters, <u>Rose Yu</u>. "Incorporating Symmetry into Deep Dynamics Models for Improved Generalization", In Proceeding of International Conference on Learning Representations (ICLR), 2021
- [C35] Fan Xie, Alex Chowdhury, Clara De Paolis, Linfeng Zhao, Lawson Wong, Rose Yu. "Deep Imitation Learning for Bimanual Robotic Manipulation" In Proceeding of Advances in Neural Information Processing Systems (NeurIPS), 2020
- [C36] Armand Comas Massague, Chi Zhang, Zlatan Feric, Octavia Camps, Rose Yu. "Learning Disentangled Representations of Video with Missing Data" In Proceeding of Advances in Neural Information Processing Systems (NeurIPS), 2020
- [C37] Jung Yeon Park, Kenneth Theo Carr, Stephan Zheng, Yisong Yue, Rose Yu "Multiresolution Tensor Learning for Efficient and Interpretable Spatial Analysis" In Proceedings of the 32th International Conference on Machine Learning (ICML), 2020
- [C38] Chintan Shah, Nima Dehmamy, Nicola Perra, Matteo Chinazzi, Albert-László Barabási, Alessandro Vespignani, Rose Yu. "Finding Patient Zero: Learning Contagion Source with Graph Neural Networks" In *International Conference on Network Science* (NetSci), 2020.

- [C39] Csaba Both, Nima Dehmamy, Albert-László Barabási, Rose Yu. "Network Layout using Graph Neural Networks" In *International Conference on Network Science* (NetSci), 2020.
- [C40] Rui Wang, Adrian Albert, Karthik, Kashinath, Mustafa, Mustafa, Rose Yu. "Towards Physics-informed Deep Learning for Spatiotemporal Modeling of Turbulent Flows", In Proceeding of ACM SIGKDD Conference on Knowledge Discovery and Data Mining (KDD), 2020
- [C41] Eliza Huang, Rui Wang, Uma Chandrasekaran, Rose Yu. "Aortic Pressure Forecasting with Deep Sequence Learning", In Proceeding of Computing in Cardiology (CinC), 2020
- [C42] Nima Dehmamy, Albert-László Barabási, Rose Yu. "Understanding the Representation Power of Graph Neural Networks in Learning Graph Topology" In Proceeding of Advances in Neural Information Processing Systems (NeurIPS), 2019
- [C43] Yukai Liu, Rose Yu, Stephan Zheng, Eric Zhan, Yisong Yue. "NAOMI: Non-Autoregressive Multiresolution Sequence Imputation" In Proceeding of Advances in Neural Information Processing Systems (NeurIPS), 2019
- [C44] Guanya Shi, Xichen Shi, Michael O'Connell, Rose Yu, Kamyar Azizzadenesheli, Anima Anand-kumar, Yisong Yue, Soon-Jo Chung. "Neural Lander: Stable Drone Landing Control using Learned Dynamics" In *International Conference on Robotics and Automation* (ICRA), 2019
- [C45] Yaguang Li, Rose Yu, Cyrus Shahabi, Yan Liu. "Diffusion Convolutional Recurrent Neural Network: Data-Driven Traffic Forecasting" In Proceedings of International Conference on Learning Representations (ICLR), 2018
- [C46] Rose Yu, Guangyu Li, Yan Liu. "Tensor regression meets Gaussian Processes." In Proceedings of International Conference on Artificial Intelligence and Statistics (AISTATS), 2018
- [C47] Rose Yu, Yaguang Li, Ugur Demiryurek, Cyrus Shahabi, Yan Liu. "Deep Learning: A Generic Approach for Extreme Condition Traffic Forecasting." In Proceedings of the Seventeenth SIAM International Conference on Data Mining (SDM), 2017
- [C48] Rose Yu, Yan Liu. "Learning from Multiway Data: Simple and Efficient Tensor Regression." In Proceedings of International Conference on Machine Learning (ICML), 2016
- [C49] Dingxiong Deng, Cyrus Shahabi, Ugur Demiryurek, Linhong Zhu, Rose Yu, Yan Liu, "Latent Space Model for Road Networks to Predict Time-Varying Traffic", In Proceeding of ACM SIGKDD Conference on Knowledge Discovery and Data Mining (KDD), 2016
- [C50] Rose Yu, Andrew Gelfand, Suju Rajan, Cyrus Shahabi, Yan Liu. "Geographic Segmentation via Latent Poisson Factor Model." In ACM International Conference on Web Search and Data Mining (WSDM), 2016
- [C51] Rose Yu, Dehua Cheng, Yan Liu. "Accelerated Online Low Rank Tensor Learning for Multivariate Spatiotemporal Streams." In Proceedings of International Conference on Machine Learning (ICML), 2015
- [C52] Rose Yu, Mohammad Taha Bahadori, Yan Liu. "Fast Multivariate Spatio-temporal Analysis via Low Rank Tensor Learning." In Proceeding of Advances in Neural Information Processing Systems (NIPS), 2014 Spotlight
- [C53] Rose Yu, Xinran He, Yan Liu. "GLAD: Group Anomaly Detection in Social Media Analysis." In ACM SIGKDD Conference on Knowledge Discovery and Data Mining (KDD), 2014
- [C54] Cuixia Gao, Naiyan Wang, Qi Yu, Zhihua Zhang. "A Feasible Nonconvex Relaxation Approach to Feature Selection." In Proceeding of 24th AAAI Conference on Artificial Intelligence (AAAI), 2011

#### JOURNAL PUBLICATIONS

- [J1] Rose Yu, Rui Wang. "Learning Dynamical Systems from Data: An Introduction to Physics-Guided Deep Learning", In Proceedings of the National Academy of Sciences 121.27 (2024): e2311808121.
- [J2] Abhimanyu Das, Weihao Kong, Andrew Leach, Shaan Mathur, Rajat Sen, <u>Rose Yu</u>. "Long-term Forecasting with TiDE: Time-series Dense Encoder", *Transactions on Machine Learning Research* (TMLR), 2023
- [J3] Mario Krenn, Lorenzo Buffoni, Bruno Coutinho, Sagi Eppel, Jacob Gates Foster, Andrew Gritsevskiy, Harlin Lee, Yichao Lu, Joao P. Moutinho, Nima Sanjabi, Rishi Sonthalia, Ngoc Mai Tran, Francisco Valente, Yangxinyu Xie, Rose Yu, Michael Kopp. "Forecasting the Future of Artificial Intelligence with Machine Learning based Link Prediction in an exponentially growing Knowledge Network". Nature Machine Intelligence 2023.
- [J4] Csaba Both, Nima Dehmamy, Rose Yu and Albert-László Barabási. "Accelerating network layouts using graph neural networks." *Nature Communications* 14, no. 1 (2023): 1560.
- [J5] Chatterjee, Ayan, Robin Walters, Zohair Shafi, Omair Shafi Ahmed, Michael Sebek, Deisy Gysi, Rose Yu, Tina Eliassi-Rad, Albert-László Barabási, and Giulia Menichetti. "Improving the generalizability of protein-ligand binding predictions with AI-Bind". Nature Communications 14, no. 1 (2023): 1989.
- [J6] Krenn, Mario, Ai, Qianxiang, Barthel, Senja, Carson, Nessa, Frei, Angelo, Frey, Nathan C, Friederich, Pascal, Gaudin, Théophile, Gayle, Alberto Alexander, Jablonka, Kevin Maik, <u>Rose Yu</u>, and others. "SELFIES and the future of molecular string representations", *Patterns* 3, no. 10 (2022): 100588.
- [J7] Utkrisht Rajkumar, Sara Javadzadeh, Mihir Bafna, Dongxia Wu, Rose Yu, Jingbo Shang, Vineet Bafna. "DeepViFi: Detecting Oncoviral Infections in Cancer Genomes using Transformers". In Proceedings of the 13th ACM International Conference on Bioinformatics, Computational Biology and Health Informatics, pp. 1-8. 2022.
- [J8] Cramer, E.Y., Lopez, V.K., Niemi, J., George, G.E., Cegan, J.C., Dettwiller, I.D., England, W.P., Farthing, M.W., Hunter, R.H., Lafferty, B. and Linkov, I., 2021. "Evaluation of individual and ensemble probabilistic forecasts of COVID-19 mortality in the US". In Proceedings of the National Academy of Sciences (PNAS), 2022
- [J9] K. Kashinath, M. Mustafa, A. Albert, J-L. Wu, C. Jiang, S. Esmaeilzadeh, K. Azizzadenesheli, R. Wang, A.Singh, A. Manepalli, D. Chirila, R.Yu, R. Walters, B. White, H. Xiao, H. A. Tchelepi, P. Marcus, A. Anandkumar, Prabhat. "Physics-informed machine learning: Case studies for weather and climate modeling" In *Journal of Philosophical Transactions of the Royal Society A*, 2020
- [J10] Rose Yu, Stephan Zheng, Anima Anandkumar, Yisong Yue. "Long Term Forecasting with Higher Order Tensor RNN". In *Journal of Machine Learning Research* (JMLR), 2018
- [J11] Rose Yu, Yan Liu. "Spatio-Temporal Analysis of Social Media Data" In Encyclopedia of GIS, 2016
- [J12] Rose Yu, Huida Qiu, Zhen Wen, Ching-Yung Liu, Yan Liu. "A Survey on Social Media Analysis Anomaly Detection" In ACM KDD Exploration, 2016
- [J13] Rose Yu, Xinran He, Yan Liu. "GLAD: Group Anomaly Detection in Social Media Analysis Extended Abstract." In ACM Transactions on Knowledge Discovery in Data (TKDD), 2015

#### AWARDED GRANTS

- [G1] PI, DARPA AIE FoundSci, GENIE: Generative Foundation Model for Automated Climate Science, \$999,306, Jan 2024 June 2025
- [G2] co-PI, CDC CFA, Epistorm: Center for Advanced Epidemic Analytics and Predictive Modeling Technology, \$17.5M (\$499,998), Oct 2023 - Sep 2028

- [G3] co-PI, DOE FES, DE-SC0024499:A Fusion Machine Learning Data Science Platform to Support the Design and Safe Operation of a Fusion Pilot Plant, \$7.4M (\$534,747), Aug 2023 July 2026
- [G4] PI, IARPA HAYSTAC Program Sub-Contract: ROMULUS and REMUS Two Systems for Building Mega-City Intelligence, \$642,745, June 2023 - June 2027
- [G5] PI, Army Research Office, ECASE: W911NF23-1-0231: Exploiting symmetry for Learning Spatiotemporal Dynamics, \$999,999, June 2023 – June 2028
- [G6] PI, NEC Faculty Research Gift Award. Physics-Guided Generative Modeling for Molecules, \$30,000, Mar 2023
- [G7] Co-PI, JSOE Early Career Faculty Development Award: AI-assisted recording of intracellular action potential waveforms from heart muscle cells, \$50,000, Jan June 2023
- [G8] Co-PI, MRPI 2023 Planning/Pilot Awards: UC Collaborative for AI-enabled Materials Exploration and Optimization (UC-CAMEO), \$299,912, Jan 2023 Jan 2025
- [G9] Co-PI, NSF IIS 2205093: SCH: MS-ADAPT: Multi-Sensor Adaptive Data Analytics for Physical Therapy, \$1,199,930, Sep 2022 Aug 2026
- [G10] PI, 2022 MICS Mini-Project, Learning to Discover Causal Graphs from Multi-Agent Spatiotemporal Data, \$17,000, Sep 2022 - Aug 2023
- [G11] PI, NSF CAREER, 2146343: New Frontiers In Large-Scale Spatiotemporal Data Analysis \$599,999, July 2022 June 2027
- [G12] PI, DoD DURIP, W911NF-22-1-0179:Computational Clusters for Robotic Deep Learning in Complex Spatiotemporal Environment, \$575,142, March 2022
- [G13] PI, NVIDIA Applied Research Accelerator Award, Accelerating Stochastic Simulation for Fast Epidemic Scenario Creation, 2 - A100 GPUs, March 2022
- [G14] Lead PI, DOE ASCR, DE-SC0022255:Discovering Physically Meaningful Structures from Climate Extreme Data \$ 3,560,504, Sep 2021 Aug 2024
- [G15] Co-PI, NSF DMS, 2134274:SCALE MoDL: Representation Theoretic Foundations of Deep Learning, \$300,000, Jan 2022 Dec 2024
- [G16] Co-PI, NSF CNS, 2100237-CCRI: ABR: Cognitive Hardware and Software Ecosystem Community Infrastructure (CHASE-CI), \$999,971, June 2021 May 2024
- [G17] Co-PI, NSF CNS, 2120019-CCRI: ENS: Cognitive Hardware and Software Ecosystem Community Infrastructure (CHASE-CI), \$1,800,000, Oct 2021 Sep 2024
- [G18] PI, Facebook Data Science Research Award, Sample-efficient sequential Bayesian decision making, \$50,000, June 2021
- [G19] PI, AWS ML Research Awards, Deep Relational Forecasting for Dynamic Graphs, \$30,000, with \$50,000 AWS Credits, Feb, 2021
- [G20] Co-PI, DARPA SBIR, W31P4Q-21-C-0014: Combining Simulated and Real Data for Near-Term Forecasting of Nonstationary Dynamic Processes, \$120,000, Feb 2021 Sep 2021.
- [G21] PI, Abiomed Research Grant, Automated Patient Care Assistant via Machine Learning, \$299,480, Nov 2020 - Oct 2023.
- [G22] PI, Army Research Office, W911NF-20-1-0334: Physics-Guided Learning for Sample Efficient Spatiotemporal Decision Making, \$370,704, Sep 2020 Aug 2023.
- [G23] PI, Adobe Data Science Research Award, Context-Aware Customer Journey Optimization in Spatiotemporal Environment, \$50,000, June 2020
- [G24] PI, Google Faculty Award, Physics Guided Deep Learning for Realistic and Efficient Traffic Simulation, \$67,694, Feb 2020
- [G25] PI, ALCF Director's Discretionary (DD) Program Allocation Award Accelerating Traffic Simulation with Graph Neural Networks, 2 million core hours, June 2020 Jan 2021.

- [G26] PI, NERSC AY 2020 Exploratory Allocation Award Physics Informed Deep Learning for Predicting Turbulence Flow, 45,000 (NERSC MPP Hours), Jan 2020 - Jan, 2021.
- [G27] PI, NSF CRII, IIS-1850349/2037745: Multiresolution Tensor Learning for Scalable and Interpretable Spatiotemporal Analysis, \$174,998, Aug, 2019 - July, 2022
- [G28] PI, Abiomed Research Grant, Anticipating Patient Outcome via Machine Learning, \$50,000, July, 2019 - Sep, 2020
- [G29] PI, ONR STTR, N68335-19-C-0310: Subcontract: Predictive Graph Convolutional Networks, \$71,784, June, 2019 - Dec, 2019
- [G30] Co-PI, Mathworks Microgrant, Battery State of Health Machine Learning Prognostics, \$17,400, Sep, 2019 - Dec, 2019
- [G31] Co-PI, ONR ECP, Subcontract: Learning and Prediction of Dynamic Processes on Evolving Networks, \$28,840, March, 2019 - Oct, 2019
- [G32] PI, Northeastern Tier 1, Physics-Informed Deep Learning for High-Resolution Climate Extremes Modeling, \$50,000, July, 2019 - Sep, 2020
- [G33] PI, Northeastern Khory Seed Grant, Learning Bimanual Robotic Manipulation Via Deep Graph Sequence, \$50,000, Aug, 2019 - Aug, 2020
- [G34] NVIDIA GPU Grant Oct 2018, 1 Titan Xp, Amazon AWS Research Credits, Oct 2018, \$20,000 Cloud Credits, Google Cloud Research Credits, Oct, 2018, \$10,000 Cloud Credits

#### Advising Postdocs Supervised

- Yadi Cao, 2024, active
- Truong Son Hy (co-advised), 2022-2023, Assistant Professor, Indiana State University
- Jedrzej Kozerawski, 2021-2022, Research Scientist, Apple
- Robin Walters, 2020-2022, Assistant Professor, Northeastern University

#### Ph.D. Students Advised

- Salva Rhling Cachay, 2022, active
- Sumanth Varambally (co-avised with Yian Ma), 2022, active
- Jianke Yang, 2022, active
- Zihao Zhou, 2022, active
- Sophia Sun, 2021, active
- Bo Zhao, 2021, active
- Dongxia (Allen) Wu (co-avised with Yian Ma), 2020, active
- Rui (Ray) Wang, 2019-2023, Postdoc at MIT

### Teaching Deep Generative Models (CSE 291)

Fall 2022, Fall 2020

Deep Reinforcement Learning (CSE 291)

Advanced Machine Learning (CS 7140)

Fall 2021

Deep Learning (CSE 151B)

Spring 2021-2023

- '

Spring 2020 Fall 2019

Special Topics in AI: Deep Learning (CS 7180)

Introduction to Computer Science Research (CS 3950)

Spring 2019

Machine Learning (CS 6140)

Fall 2018

# INVITED TALK Year 2024

Keynote Speaker, ICML workshop on Geometry-grounded representation learning	July, 2024
Physics Colloquium, UCSD Physics Department	April, 2024
Invited Speaker, Learning Collective Variables and Coarse Grained Models, IMSI	April, 2024
Invited Speaker, AI4Science Seminar, Amazon Science	Jan, 2024
Year 2023	
Keynote Speaker, KDD workshop on Uncertainty Quantification and Reasoning	Aug 2023
Keynote Speaker, KDD workshop on Data Science for Social Good	Aug 2023
Keynote Speaker, Learning for Dynamics and Control (L4DC)	June 2023
Keynote Speaker, MATH $+X$ 2023 Symposium, Simons Foundation	May 2023
Invited Speaker, Flatiron Institute	Mar 2023
Columbia LEAP Center, Columbia University	Mar 2023
Princeton Center of Statistic and Machine Learning, Princeton University	Mar 2023
Invited Speaker, IPAM Workshop "Learning and Emergence in Molecular Systems"	Jan 2023
Year 2022	
Keynote Speaker, NeurIPS 2022 Tackling Climate Change with ML Workshop	Dec 2022
NeurIPS 2022: "The Symbiosis of Deep Learning and Differential Equations II",	Dec 2022
UCR Computer Science Colloquium, UC Riverside	Oct 2022
Tensor Methods and Applications to Real-World Data, SIAM MDS	Sep 2022
Challenges and Prospects of ML for the Physical Sciences, Flatiron Institute	June 2022
Aspen Workshop on Machine Learning and Earth System Models	June 2022
Physics Informed Machine Learning conference, Los Alamos National Lab	May 2022
Ames Lab, Scientific Machine Learning: Foundations and Applications	April 2022
RIKEN, Predictive Science Seminar	Jan 2022
John Hopkins University 2022 TRIPODS Winter School	Jan 2022
Year 2021	
Keynote Speaker, KITP Machine Learning for Climate Conference	Nov 2021

University of Washington, Data-Driven Methods for Science and Engineering Seminar	Oct 2021
Caltech Explainable AI Virtual Workshop	Sep 2021
CMU AI in Physics seminar	Sep 2021
Georgia Tech Applied & Computational Math	Sep 2021
KDD Lecture Style Tutorial	August 2021
NASA Glenn Research Center	July 2021
One World MINDS Seminar	July 2021
RIKEN AIP Seminar, Japan	June 2021
Institute for Pure & Applied Mathematics (IPAM), UCLA	May 2021
AI Seminar, USC/ISI	May 2021
CRUNCH Applied Math Group, Brown University	April 2021
Featured Talk at NVIDIA GTC 2021	March 2021
Applied Math Department Colloquium, University of Arizona	Feb 2021
Duke University, Deep Learning Reading Group	Feb 2021
Oak Ridge National Laboratory Workshop on AI for Robust Engineering & Science	Jan 2021
Year 2020	
Machine Learning in Science and Engineering virtual conference	Dec 2020
NeurIPS 2020 Workshop on Quantum Tensor Networks	Dec 2020
NeurIPS 2020 Workshop on AI for Earth	Dec 2020
NeurIPS 2020 Workshop on Interpretable Inductive Biases	Dec 2020
AGU Fall Meeting Invited Talks	Dec 2020
Caltech Climate Modeling Alliance (CliMA) group	Nov 2020
AAAI 2020 Symposium on Physics-Guided AI for Accelerating Scientific Discovery	Nov 2020
LA Life Science Summit	Oct 2020
COVID-19 Forecast Hub	Sep 2020
International School and Conference on Network Science	Sep 2020
ODSC Europe 2020 Virtual Conference	Sep 2020

Mathematics of Data Science Virtual Lecture Series, Tufts, MA	June 2020
Facebook Artificial Intelligence Research, Menlo Park, CA	April 2020
Functional Data over Multidimensional Domain, EPFL, Switzerland,	April 2020
AI for Robust Engineering and Science workshop, Oak Ridge National Lab	Jan 2020
Physics Informed Machine Learning workshop, Los Alamos National Lab	Jan 2020
Year 2019	
Mitsubishi Electric Research Laboratories (MERL), Cambridge	Oct 2019
Plenary Speaker, European Research Network on System Identification	Sep, 2019
Hazy Research Group Seminar, Stanford University	August 2019
KDD 2019 Tensor Methods Workshop, Anchorage	August 2019
University of Connecticut, Connecticut	July 2019
Google Research, Mountain View	July 2019
Machine Learning Theory Workshop, Peking University, China	June 2019
Auto Lab, University of Michigan, Ann Arbor	May 2019
CLR 2019 Workshop on Deep Generative Models, New Orleans	May 2019
Tensor Working Group on Simons Foundation, New York	May 2019
Workshop Low-rank Optimization and Applications, Leipzig, Germany	April 2019
Young European Probabilists XV workshop, Eindhoven, Netherland	March 2019
Lawrence Berkeley National Laboratory (LBNL)	March 2019
Year 2018	
Amazon Research, Palo Alto	Dec 2018
Salesforce Research, Palo Alto,	Dec 2018
Machine Learning Group Seminar, Harvard,	Nov 28 2018
Clinical Machine Learning Group Seminar, MIT,	Nov 13 2018
Keynote Speaker, Climate Informatics 2018 (CI 2018),	Sep 2018
Henry L. Pierce Laboratory Seminar Series, MIT,	Sep 12, 2018
Japan RIKEN Center for Advanced Intelligence Project (AIP), Tokyo,	July 3, 2018

Disney Research, Burbank,	May 22, 2018
Year 2017	
Department of Management Science, University of Miami	Nov 18, 2017

Center of Data Science, New York University

March 30, 2017

Oct 6, 2017

Department of Computer Science, Brown University

March 13, 2017

School of Industrial and Systems Engineering, Georgia Institute of Technology March 6, 2017

College of Computer and Information Science, Northeastern University

March 3, 2017

AI with The Best, Online Conference Sep 17, 2016

Computer Science Department, Stanford University

May 23, 2016

#### ACADEMIC SERVICE Conference Organizing Committee

Program Chair, ICLR (2025)

Workshop Chair, NeurIPS (2024)

Industry Expo Chair, ICML (2023, 2022)

Workshop Chair, ICLR (2023)

Poster Chair, KDD (2020)

Proceedings Chair, ACM SIGSPATIAL (2020)

KITP: At the Crossroad of Physics and Machine Learning, 2019

Department of Computing and Mathematical Sciences, Caltech

Proceedings Chair, WSDM (2018)

Short Paper Chair, CIKM (2017)

#### Senior Program Committee (or Area Chair)

L4DC (2024), NeurIPS (2020-2024), ICML(2020-2022), ICLR (2023, 2022, 2021), AAAI (2021), IJCAI (2020), SDM (2020)

#### Workshop Organizing Committee

ICML Time Series Workshop, (2021, 2019, 2017)

ICCV Simulation Technology for Embodied AI, 2021

ICLR Workshop on Deep Learning for Simulation (2021)

NeurIPS Workshop on Machine Learning for Engineering (2020)

NIPS Woman in Machine Learning Workshop (2016)

NIPS workshop on Learning with Tensors: Why Now and How? (2016)

## **Program Committee**

ICML (2020, 2019, 2018), NeurIPS (2019, 2018), ICLR (2020, 2019), KDD (2019), AISTATS (2020, 2019), SDM (2019), AAAI (2018), IJCAI (2018), CIKM (2017), NIPS Time Series Workshop (2016), ICML Time Series Workshop (2016)

# Grant Reviewer/Panelist

Department of Energy (DOE) Review Panel (2019-2023) National Science Foundation (NSF) Review Panel (2018-2022)

## Reviewer

AAAI 2021 Spring Symposium on Combining Machine Learning with Physical Sciences, Proceedings of IEEE (2019), Journal of Machine Learning Research (JMLR), Journal of Artificial Intelligence Research (JAIR), Transactions on Knowledge Discovery from Data (TKDD), IEEE Transactions on Knowledge and Data Engineering (TKDE), IEEE Intelligent Transportation Systems Transaction (ITS)