

Liping Liu

POSITION	Associate Professor Department of Computer Science, Tufts University JCC 367, 177 College Ave., Medford, MA 02155 <i>Email:</i> liping.liu@tufts.edu <i>Phone:</i> +1-617-627-0556 <i>Website:</i> https://www.eecs.tufts.edu/~liulp/
RESEARCH INTERESTS	Probabilistic modeling, Generative models, Biochemical data analysis, Simulation of fluid dynamics, Graph data modeling,
EXPERIENCE	2024 – present, Associate Professor, Tufts University 2022 – 2024, Assistant Professor, Tufts University 2017 – 2022, The Schwartz Family Assistant Professor, Tufts University 2016 – 2017, Visiting assistant professor, Tufts University 2016 – 2017, Postdoctoral researcher, Columbia University 2015 summer, Research intern, IBM T.J. Watson Research 2009 – 2010, Developer, Alibaba
EDUCATION	Ph.D., Oregon State University , 2016 Thesis: <i>Machine learning methods in computational sustainability</i> Advisor: Thomas G. Dietterich M.S., Nanjing University , 2009 Thesis: <i>Fast feature extraction and incremental dimensionality reduction based on machine learning techniques</i> Advisor: Yuan Jiang B.S., Hebei University of Technology , 2006
PUBLICATIONS	Peer-reviewed Conference papers Panagiotis Lymperopoulos and Li-Ping Liu . Graph pruning for enumeration of minimal unsatisfiable subsets. In <i>The 27th International Conference on Artificial Intelligence and Statistics</i> . PMLR, 2024 (AISTATS’2024) Luning Sun, Xu Han, Han Gao, Jian-Xun Wang, and Li-Ping Liu . Unifying predictions of deterministic and stochastic physics in mesh-reduced space with sequential flow generative model. In <i>Thirty-seventh Conference on Neural Information Processing Systems</i> , 2023 (Neurips’2023 Spotlight) Xiaohui Chen, Yinkai Wang, Yuanqi Du, Soha Hassoun, and Li-Ping Liu . On separate normalization in self-supervised transformers. In <i>Thirty-seventh Conference on Neural Information Processing Systems</i> , 2023 (Neurips’2023) Xiaohui Chen, Jiankai Sun, Taiqing Wang, Ruocheng Guo, Li-Ping Liu , and Anan Zhang. Graph-based model-agnostic data subsampling for recommendation systems. In <i>29th SIGKDD Conference on Knowledge Discovery and Data Mining - Applied Data Science Track</i> , 2023 (KDD’2023) Xiaohui Chen, Jiaxing He, Xu Han, and Li-Ping Liu . Efficient and degree-guided graph generation via discrete diffusion modeling. In <i>International Conference on Machine Learning</i> . PMLR, 2023 (ICML’2023)

- Han Gao, Xu Han, Jiaoyang Huang, Jian-Xun Wang, and **Li-Ping Liu**. PatchGT: Transformer over non-trainable clusters for learning graph representations. In *Learning on Graphs Conference*, pages 27–1. PMLR, 2022 (LoG’2022)
- Linfeng Liu, Michael C Hughes, Soha Hassoun, and **Li-Ping Liu**. Stochastic iterative graph matching. In *International Conference on Machine Learning*, pages 6815–6825. PMLR, 2021 (ICML’2021)
- Xiaohui Chen, Xu Han, Jiajing Hu, Francisco Ruiz, and **Li-Ping Liu**. Order matters: Probabilistic modeling of node sequence for graph generation. In *International Conference on Machine Learning*, pages 1630–1639. PMLR, 2021 (ICML’2021)
- Xu Han, Xiaohui Chen, and **Li-Ping Liu**. Gan ensemble for anomaly detection. In *Proceedings of the AAAI Conference on Artificial Intelligence*, volume 35, pages 4090–4097, 2021 (AAAI’2021)
- Christopher M Polleys, Panagiotis Lymperopoulos, Hong-Thao Thieu, Elizabeth Genega, **Li-Ping Liu**, and Irene Georgakoudi. Deep-learning-based image restoration of depth-resolved, label-free, two-photon images for the quantitative morphological and functional characterization of human cervical tissues. In *Imaging, Manipulation, and Analysis of Biomolecules, Cells, and Tissues XIX*, volume 11647, page 116470Z. SPIE, 2021
- Linfeng Liu and **Li-Ping Liu**. Localizing and amortizing: Efficient inference for gaussian processes. In *Asian Conference on Machine Learning*, pages 823–836. PMLR, 2020 (ACML’2020)
- Gabriel Appleby, Linfeng Liu, and **Li-Ping Liu**. Kriging convolutional networks. In *Proceedings of the AAAI Conference on Artificial Intelligence*, volume 34, pages 3187–3194, 2020 (AAAI’2020)
- Linfeng Liu and **Li-Ping Liu**. Amortized variational inference with graph convolutional networks for gaussian processes. In *The 22nd International Conference on Artificial Intelligence and Statistics*, pages 2291–2300. PMLR, 2019 (AISTATS’2019)
- Li-Ping Liu**, Francisco Ruiz, Susan Athey, and David Blei. Context selection for embedding models. *Advances in Neural Information Processing Systems*, 30, 2017 (Neurips’2017)
- Li-Ping Liu** and David M Blei. Zero-inflated exponential family embeddings. In *International Conference on Machine Learning*, pages 2140–2148. PMLR, 2017 (ICML’2017)
- Li-Ping Liu**, Thomas G Dietterich, Nan Li, and Zhi-Hua Zhou. Transductive optimization of top k precision. In *Proceedings of the Twenty-Fifth International Joint Conference on Artificial Intelligence*, pages 1781–1787, 2016 (IJCAI’2016)
- Yuanli Pei, **Li-Ping Liu**, and Xiaoli Z Fern. Bayesian active clustering with pairwise constraints. In *Machine Learning and Knowledge Discovery in Databases: European Conference, ECML PKDD 2015, Porto, Portugal, September 7-11, 2015, Proceedings, Part I 15*, pages 235–250. Springer, 2015 (ECML/PKDD’2015)
- Li-Ping Liu**, Daniel Sheldon, and Thomas Dietterich. Gaussian approximation of collective graphical models. In *International Conference on Machine Learning*, pages 1602–1610. PMLR, 2014 (ICML’2014)
- Li-Ping Liu** and Thomas Dietterich. Learnability of the superset label learning problem. In *International Conference on Machine Learning*, pages 1629–1637. PMLR, 2014 (ICML’2014)
- Li-Ping Liu** and Thomas Dietterich. A conditional multinomial mixture model for superset label learning. *Advances in neural information processing systems*, 25, 2012 (Neurips’2012)
- Li-Ping Liu** and Xiaoli Z Fern. Constructing training sets for outlier detection. In

Proceedings of the 2012 SIAM International Conference on Data Mining, pages 919–929. SIAM, 2012 (SDM’2012)

Rebecca Hutchinson, **Li-Ping Liu**, and Thomas Dietterich. Incorporating boosted regression trees into ecological latent variable models. In *Proceedings of the AAAI Conference on Artificial Intelligence*, volume 25, pages 1343–1348, 2011 (AAAI’2011)

Li-Ping Liu, Yuan Jiang, and Zhi-Hua Zhou. Least square incremental linear discriminant analysis. In *2009 Ninth IEEE International Conference on Data Mining*, pages 298–306. IEEE, 2009 (ICDM’2009)

Li-Ping Liu, Yang Yu, Yuan Jiang, and Zhi-Hua Zhou. Tefe: A time-efficient approach to feature extraction. In *2008 Eighth IEEE International Conference on Data Mining*, pages 423–432. IEEE, 2008 (ICDM’2008)

Journal papers

Xinmeng Li, Yan Zhou Chen, Apurva Kalia, Hao Zhu, **Li-Ping Liu**, and Soha Hassoun. An ensemble spectral prediction (esp) model for metabolite annotation. *Bioinformatics*, 40(8):btac490, 2024

Han Gao, Xu Han, Xiantao Fan, Luning Sun, **Li-Ping Liu**, Lian Duan, and Jian-Xun Wang. Bayesian conditional diffusion models for versatile spatiotemporal turbulence generation. *Computer Methods in Applied Mechanics and Engineering*, 427:117023, 2024

Shivam Goel, Panagiotis Lymperopoulos, Ravenna Thielstrom, Evan Krause, Patrick Feeney, Pierrick Lorang, Sarah Schneider, Yichen Wei, Eric Kildebeck, Stephen Goss, Michael C. Hughes, **Li-Ping Liu**, Jivko Sinapov, and Matthias Scheutz. A neurosymbolic cognitive architecture framework for handling novelties in open worlds. *Artificial Intelligence*, page 104111, 2024

Xu Han, Xiaohui Chen, Francisco JR Ruiz, and **Li-Ping Liu**. Fitting autoregressive graph generative models through maximum likelihood estimation. *Journal of Machine Learning Research*, 24(97):1–30, 2023 (JMLR’2023)

Patrick Feeney, Sarah Schneider, Panagiotis Lymperopoulos, **Li-Ping Liu**, Matthias Scheutz, and Michael C Hughes. Novelcraft: A dataset for novelty detection and discovery in open worlds. *Transactions on Machine Learning Research*, 2023 (TMLR’2023)

Vladimir Porokhin, **Li-Ping Liu**, and Soha Hassoun. Using graph neural networks for site-of-metabolism prediction and its applications to ranking promiscuous enzymatic products. *Bioinformatics*, 39(3), 2023

Xiaohui Chen, Xi Chen, and **Li-Ping Liu**. Interpretable node representation with attribute decoding. *Transactions on Machine Learning Research*, 2022 (TMLR’2022)

Linfeng Liu, Xu Han, Dawei Zhou, and **Li-Ping Liu**. Towards accurate subgraph similarity computation via neural graph pruning. *Transactions on Machine Learning Research*, 2022 (TMLR’2022)

Xinmeng Li, **Li-Ping Liu**, and Soha Hassoun. Boost-RS: Boosted embeddings for recommender systems and its application to enzyme–substrate interaction prediction. *Bioinformatics*, 38(10):2832–2838, 2022

Julie Jiang, **Li-Ping Liu**, and Soha Hassoun. Learning graph representations of biochemical networks and its application to enzymatic link prediction. *Bioinformatics*, 37(6):793–799, 2021

Ramtin Hosseini, Neda Hassanpour, **Li-Ping Liu**, and Soha Hassoun. Pathway-activity likelihood analysis and metabolite annotation for untargeted metabolomics using probabilistic modeling. *Metabolites*, 10(5):183, 2020

Workshop papers

Yukun Li and **Li-Ping Liu**. Enhancing diffusion-based point cloud generation with smoothness constraint. In *NeurIPS 2023 Workshop on Diffusion Models*, 2023

Xiaohui Chen, Mingyang Wu, and **Li-Ping Liu**. EDGE++: Improved training and sampling of EDGE. In *NeurIPS 2023 Workshop: New Frontiers in Graph Learning*, 2023

Panagiotis Lymperopoulos, Yukun Li, and **Li-Ping Liu**. Exploiting variable correlation with masked modeling for anomaly detection in time series. In *NeurIPS 2022 Workshop on Robustness in Sequence Modeling*, 2022

Hao Zhu, **Li-Ping Liu**, and Soha Hassoun. Using graph neural networks for mass spectrometry prediction. In *Machine Learning in Computational Biology*, 2020 (MLCB'2020)

INVITED TALKS / PRESENTATIONS

08/16/2024, Graph Learning: A Versatile Tool for Physics Simulations. *CIRC 2024–2025 Symposium Series*, U of Rochester.

03/13/2024, Generative models for graph data: probability calculations and efficiency. *Seminar*, Google DeepMind.

11/08/2023, Generative models for graph data: probability calculations and efficiency. *AIR seminar*, Boston University

10/30/2023, The new frontier of graph generation. *CS seminar*, Brandeis University

03/20/2023, Understanding biochemical reactions using graph neural networks. *Sanghani Center for AI and Analytics Seminar Series*, Virginia Tech

02/14/2023, Address combinatorial graph problems with learning methods, *IAIFI Journal Club*, MIT

10/07/2022, The MLE principle in autoregressive graph generation, *CS/DS Colloquium*, WPI

03/25/2022, The MLE principle in autoregressive graph generation, *NE Tripods Workshop*, Tufts

12/03/2021, Probabilistic methods for graph learning, *(virtual) a seminar at Prof. Wei Wang's lab*, UCLA

08/30/2021, The MLE principle in autoregressive graph generation, *(virtual) a seminar at the iSAIL Lab*, UIUC

09/13/2018, Embedding: choose right relations to embed, *CS Graduate Seminar*, UMass Amherst

09/29/2017, Zero-inflated exponential family embeddings, *CS/DS Colloquium*, WPI

FUNDING

04/01/2023 – 03/31/2028, Single PI, NSF, CAREER: New Frontiers in Graph Generation, \$556,357

11/14/2022 – 11/13/2023, Co-PI (PI: Thomas Schnelldorfer), Tufts DISC Seed Grant Program, Computer-Assisted Laparoscopic Identification of Non-Cirrhotic Liver Disease, \$25,000

10/01/2019 – 09/30/2024, Co-PI (PI: Soha Hassoun), NSF, FET: Small: Tools and Experimental Validation for Predicting Enzymatic Promiscuity and its Products, \$631,393

09/23/2019 – 08/31/2023, Co-PI (PI: Soha Hassoun), NIH, R01: Computational Techniques for Advancing Untargeted Metabolomics Analysis, \$1,250,000

09/01/2020 – 08/31/2021, Co-PI (PI: Soha Hassoun), NIH, R03: Using Machine Learning Techniques to Characterize the Metabolomics Workbench Dataset, \$263,120

07/01/2020 – 06/30/2021, Co-PI (PI: Irene Georgakoudi). Tufts DISC Seed Grant Program, Data Science Methods to Enable Label-free, Morphofunctional Imaging in Human Tissue, \$12,725

10/01/2019 – 03/31/2023, Co-PI (PI: Matthias Scheutz), DARPA, ACT-NOW: Autonomous Cognitive Technologies for Novelty in Open Worlds, \$6,737,932

10/01/2019 – 09/30/2022, PI (Co-PIs: Michael Hughes and Thomas Stopka) NSF, CISE RI: Small: Amortized Inference for Large-Scale Graphical Models, \$399,923

08/01/2019 – 05/31/2021, PI (Contact PI: Thomas Schnelldorfer), NIH, R03: Development of Deep Neural Networks for Automated Detection of Cancer Metastases in Staging Laparoscopy Images. \$154,900

03/15/2019 – 02/28/2021, Single PI, NSF, CRII: RI: Self-Attention through the Bayesian Lens, \$174,980

07/01/2018 – 06/30/2019, Co-PI (PI: Jonathan Lamontagne), Tufts Collaborates Round VIII, Can Machine Learning Improve the Representation of Humans in the Hydrologic Cycle?, \$47,191

EXTERNAL SERVICE

- Session chair
 - AAAI Conference on Artificial Intelligence (AAAI), 2023
 - International Conference on Artificial Intelligence and Statistics (AISTATS), 2022
- Senior program committee member/Area chair
 - AAAI Conference on Artificial Intelligence (AAAI), 2019, 2022 – 2024
 - AAAI-24's Special Track on AI for Social Impact, 2024
 - International Joint Conference on Artificial Intelligence (IJCAI), 2021 – 2024
 - International Conference on Artificial Intelligence and Statistics (AISTATS), 2022 – 2024
- Program committee member/Reviewer
 - International Joint Conference on Artificial Intelligence (IJCAI), 2015 – 2020, 2023
 - AAAI Conference on Artificial Intelligence (AAAI), 2017, 2018, 2020, 2021
 - International Conference on Learning Representations (ICLR), 2019 – 2024
 - International Conference on Machine Learning (ICML), 2017 – 2021, 2023
 - Neural Information Processing Systems (Neurips), 2017 – 2024
 - International Conference on Artificial Intelligence and Statistics (AISTATS), 2018, 2021
- NSF panelist, 2017, 2021
- Reviewer
 - Journal of Machine Learning Research (JMLR)
 - IEEE Transactions on Knowledge and Data Engineering (TKDE)
 - IEEE Transactions on Pattern Analysis and Machine Intelligence (PAMI)

- Journal of Artificial Intelligence Research (JAIR)
 - International Journal of Computer Vision (IJCV)
- Judge for Massachusetts Region IV Science Fair (judging scientific projects conducted by high school students), 2019 – 2024

ADVISING

- PhD students
 - Linfeng Liu, PhD, 09/2017 – 05/2022. Dissertation: *Learning from relational data via graph neural networks*
 - Xu Han, PhD candidate, 09/2020 – . Research topic: *Predicting dynamic systems with graph neural networks*
 - Jiajing Hu, PhD student, 09/2020 – . Research topic: *Deep inference methods for time series modeling*
 - Yukun Li, PhD candidate, 01/2021 – . Research topic: *Hybrid energy-based probabilistic models*
 - Xiaohui Chen, PhD candidate, 09/2021 – . Research topic: *Graph generative models and maximum likelihood estimation*
 - Panagiotis Lympieropoulos, PhD candidate, 09/2021 – . Research topic: *A probabilistic approach to neural-symbolic learning*
 - Jacob Boerma, PhD student, 09/2023 – . Research topic: *TBD*

TEACHING

2024 Spring, CS 135 Introduction to Machine Learning
 2023 Fall, CS 137 Deep Neural Networks
 2023 Spring, CS 150 Deep Graph Learning
 2022 Fall, CS 137 Deep Neural Networks
 2021 Fall, CS 137 Deep Neural Networks
 2020 Fall, COMP 137 Deep Neural Networks
 2019 Fall, COMP 150 Machine Learning for Graph Analytics
 2019 Spring, COMP 150 Deep Neural Networks
 2018 Fall, COMP 135 Introduction to Machine Learning
 2018 Spring, COMP 135 Introduction to Machine Learning
 2017 Fall, COMP 150 Machine Learning for Ecology and Sustainability

INTERNAL SERVICES

- Department services
 - Graduate committee, 2020 – 2023
 - Curriculum Committee, 2023 – 2024
 - Co-organizing department colloquium series, 2021 – 2022, 2023 – 2024
 - MSCS oversight committee, 2020 – 2021
 - MSDS admission committee, 2023 – 2024
 - Graduate admission committee, 2018 – 2020
 - Search committee 2019, 2024
 - Interviewer for the DISC director search, 2018 – 2019
- School and university services
 - University, Information Technology Committee, 2019 – 2024
 - School of Engineering, Academic Standing Committee, 2019 – 2024

- School of Engineering, Strategic Planning (Graduate education group), 2017 – 2018