# Liping Liu

#### Position Assistant Professor

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## RESEARCH Interests

Probabilistic modeling, Statistical inference, Generative models, Graph neural networks, Graph data modeling, Biochemical data analysis, Anomaly detection

#### EXPERIENCE

2022 – present, 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: Machine learning methods in computational sustainability. Advisor: Thomas G. Dietterich

# M.S., Nanjing University, 2009

Thesis: Fast feature extraction and incremental dimensionality reduction based on machine learning techniques. Advisor: Yuan Jiang

B.S., Hebei University of Technology, 2006

# Publications

## Journal papers

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

# Peer-reviewed Conference papers

Xiaohui Chen, Jiankai Sun, Taiqing Wang, Ruocheng Guo, **Li-Ping Liu**, and Aonan Zhang. Graph-based model-agnostic data subsampling for recommendation systems. In 29th SIGKDD Conference on Knowledge Discovery and Data Mining - Applied Data Science Track, 2023 (KDD'2023)

Xiaohui Chen, Jiaxing He, Xu Han, and **Li-Ping Liu**. Efficient and degree-guided graph generation via discrete diffusion modeling. In *International Conference on Machine Learning*. 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 depthresolved, 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)

## Workshop papers

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

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

 $02/14/2023,\,\mathrm{Address}$  combinatorial graph problems with learning methods,  $\mathit{IAIFI}$   $\mathit{Journal}$   $\mathit{Club},\,\mathrm{MIT}$ 

 $10/07/2022,\, {\rm The}$  MLE principle in autoregressive graph generation,  $\mathit{CS/DS}$  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,  $\mathit{CS}$   $\mathit{Graduate}$   $\mathit{Seminar},$  UMass Amherst

#### 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, \$399,923.00.

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

- o AAAI Conference on Artificial Intelligence (AAAI), 2023
- International Conference on Artificial Intelligence and Statistics (AISTATS), 2022
- Senior program committee member
  - o AAAI Conference on Artificial Intelligence (AAAI), 2019, 2022, 2023
  - o International Joint Conference on Artificial Intelligence (IJCAI), 2021, 2022
  - International Conference on Artificial Intelligence and Statistics (AISTATS), 2022, 2023
- Program committee member/reviewer
  - International Joint Conference on Artificial Intelligence (IJCAI), 2015 2020, 2023
  - o AAAI Conference on Artificial Intelligence (AAAI), 2017, 2018, 2020, 2021
  - o International Conference on Learning Representations (ICLR), 2019 2023

- International Conference on Machine Learning (ICML), 2017 2021, 2023
- Neural Information Processing Systems (Neurips), 2017 2023
- International Conference on Artificial Intelligence and Statistics (AISTATS), 2018, 2021
- NSF panelist, 2017, 2021

#### Reviewer

- o Journal of Machine Learning Research (JMLR)
- o IEEE Transactions on Knowledge and Data Engineering (TKDE)
- o IEEE Transactions on Pattern Analysis and Machine Intelligence (PAMI)
- o 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, 2020, 2021, 2023

#### 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
- $\circ$  Jiajing Hu, PhD student, 09/2020 . Research topic: Deep inference methods for time series modeling
- $\circ$  Yukun Li, PhD candidate, 01/2021 . Research topic: Hybrid energy-based probabilistic models
- $\circ$  Xiaohui Chen, PhD candidate, 09/2021 . Research topic: Graph generative models and maximum likelihood estimation
- $\circ$  Panagiotis Lymperopoulos, PhD candidate, 09/2021 . Research topic: A probabilistic approach to neural-symbolic learning

### • Master students

- Jiaxing He, 08/2023 (expected). Thesis: An explainable message-passing method for subgraph matching
- $\circ$  Changhao Li, 08/2023 (expected). The sis: A neural method for frequent graph pattern searching
- Ruiyuan Gu, MS, 05/2022. Thesis: Ladder polynomial neural networks
- Daniel Dinjian, MS, 05/2019. Thesis: Bayesbigan and ganify research and a developer tool for generative adversarial networks

#### • Undergraduates

- $\circ\,$  Brawner Quan, on the project of text data analysis, 2021 2022
- Kyle Sayers, on the project of medical image classification, 2021 2022
- o Julie, Jiang, on the project of metabolic network analysis, 2018 2019
- o Duc Nguyen, on the project of medical image classification, 2019 2020

# TEACHING

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
- o Organizing (with Raja Sambasivan) department colloquium series, 2021 2022
- o MSCS oversight committee, 2020 2021
- Graduate admission committee, 2018 2020
- $\circ$  Search committee 2018 2019
- o 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

# • Academic advising

- Undergraduates: advising 20+ undergraduates annually
- Master students: advising 5+ master students annually

### • Dissertation committee member

- Shivam Goel (advisee of Jivko Sinapov)
- o Zirui Fu (ECE Department, advisee of Marco Donato)
- o Tiffani Hui (Chemistry Department, advisee of Yu-Shan Lin)
- o Kapil Devkota (advisee of Lenore Cowen), graduated Summer 2023
- o Xinmeng Li (advisee of Soha Hassoun), graduated Spring 2022
- o Xin Dai (WPI, advisee of Xiangnan Kong), graduated Spring 2022
- o Alireza Alizadeh (ECE Department, advisee of Vu Mai), graduated Spring 2021
- o Zhaokun Xue (advisee of Alva Couch), graduated Spring 2021
- o Saeed Majidi (advisee of Gregory Crane), graduated Fall 2020
- o Rafia Malik (ECE Department, advisee of Mai Vu), graduated Fall 2019
- o Hao Cui (advisee of Roni Khardon), graduated Spring 2019
- Long Bao (ECE Department, advisee of Karen Panetta), graduated Spring 2019
- o Sepideh Sadeghi (advisee of Matthias Scheutz), graduated Fall 2018
- o Rishit Sheth (advisee of Roni Khardon), graduated Fall 2018
- Weitong Ruan (ECE Department, advisee of Eric Miller), graduated Summer 2018
- o Neda Hassanpour (advisee of Soha Hassoun), graduated Spring 2018

### • Qualifying exam committee member

- o Margaret Martin (advisee of Soha Hassoun), Spring 2023
- Frederick Zhang (advisee of Soha Hassoun), Spring 2023
- o Patrick Feeney (advisee of Michael Hughes), Fall 2022
- o Vlad Porokhin (advisee of Soha Hassoun), Spring 2022
- o Apurva Kalia (advisee of Soha Hassoun), Spring 2022
- o Kyle Heuton (advisee of Michael Hughes), Spring 2022

- $\circ\,$  Preetish Rath (advisee of Michael Hughes), Fall 2021
- o Hao Zhu (advisee of Soha Hassoun), Spring 2021
- $\circ\,$  Sophia Sklaviadis (advisee of J.P. de Ruiter), Fall 2020
- o Xinmeng Li (advisee of Soha Hassoun), Fall 2020
- o Zhaokun Xue (advisee of Alva Couch), Fall 2018