RENMING (REMY) LIU

4902 Forbes Ave Rm 7401, Pittsburgh, PA 15213

RESEARCH INTERESTS

- Network Biology
- Graph Representation Learning
- AI for Health & Science
- Single-Cell Analysis

EDUCATION

Michigan State University

09/2019 - 05/2024

Ph.D., Computational Mathematics, Science and Engineering

Michigan State University

09/2014 - 06/2018

B.S., Chemical Engineering

Concentration in Biochemical Engineering

Minor in Computer Science

PROFESSIONAL EXPERIENCE

Post-doctoral Fellow

06/2024 - present

Ray and Stephanie Lane Computational Biology Department. Carnegie Mellon University.

Topic: Machine learning methods and software for single-cell epigenomics.

Ph.D. Student and Research Assistant

09/2019 - 05/2024

Department of Computational Mathematics, Science and Engineering. Michigan State University.

Topic: Biomedical and Molecular Interaction Networks, Graph Representation Learning, Spectral Graph Theory.

Research Assistant 06/2023 - 08/2023

Department of Biomedical Informatics. Colorado University Anschutz Medical Campus.

Topic: Context-specific biological network embeddings.

Research Assistant 05/2017 - 08/2019

Department of Chemical Engineering and Materials Science. Michigan State University.

Topic: Thermodynamic modeling of associating systems including alcohols and acetic acids.

Professional Aide 09/2018 - 08/2019

Department of Computational Mathematics, Science and Engineering. Michigan State University.

Topic: Human gene function prediction using ML with biological networks.

HONORS & AWARDS

Silver Medal in Kaggle

2022

NeurIPS Multimodal Single-Cell Integration Across Time, Individuals, and Batches.

Outstanding Graduate Student Award

2022

Awarded to the most outstanding doctoral student in each program.

Raymond P. and Marie M. Ginther Fellowship

2019

Awarded to outstanding incoming Ph.D. students to the CMSE program at MSU.

Maurice G. and Sara V. Larian Scholarship

2017

OPEN-SOURCE PROJECTS

OBNB (sole developer)

2023

A Python toolkit for benchmarking biomedical networks using gene annotation resources.

DANCE (core developer)

2022

An extensive deep learning toolkit for single-cell (multi-)omics data.

PvGenePlexus

2022

A network-based gene classification service using ML with gene interaction network features.

PecanPy (sole developer)

2020

A memory efficient and parallel Python implementation of node 2 vec with an improved version node 2 vec for weighted graph.

PUBLICATIONS

*indicates (co-)first author

Journal and Conference Papers

- Graph Positional and Structural Encoder
 S. Cantürk*, R. Liu*, O. Lapointe-Gagné, V. Létourneau, G. Wolf, D. Beaini, L. Rampášek International Conference on Machine Learning (ICML), 2024
- DANCE: A Deep Learning Library and Benchmark Platform for Single-cell Analysis J. Ding*, H. Wen*, W. Tang*, R. Liu*, Z. Li, J. Venegas, R. Su, D. Molho, W. Jin, W. Zou, Y. Wang, R. Yang, Y. Xie, J. Tang

 Genome Biology, 2024
- Deep Learning in Single-Cell Analysis
 D. Molho*, J. Ding, Z. Li, H. Wen, W. Tang, Y. Wang, J. Venegas, W. Jin, R. Liu, R. Su, P. Danaher, R. Yang, Y. Lei, Y. Xie, J. Tang
 ACM Transactions on Intelligent Systems and Technology, 2024
- Joint representation of molecular netowrks from multiple species improves gene classification C.A. Mancuso*, K.A. Johnson, R. Liu, A. Krishnan PLOS Computational Biology, 2024
- SpatialCTD: a large-scale TME spatial transcriptomic dataset to evaluate cell type deconvolution for immuno-oncology
 J. Ding*, J. Venegas, Q. Lu, Y. Wang, W. Jin, H. Wen, R. Liu, W. Tang, Z. Li, W. Zuo, Y. Chang, Y. Lei, P. Danaher, Y. Xie, J. Tang
 Journal of Computational Biology, 2024
- Open Biomedical Network Benchmark: A Python Toolkit for Generating Benchmakring Datasets with Biomedical Networks

R. Liu*, A. Krishnan

Machine Learning in Computational Biology (MLCB). PMLR, 2023

- Single-Cell Multimodal Prediction via Transformers
 W. Tang*, H. Wen*, R. Liu*, J. Ding, W. Jin, Y. Xie, H. Liu, J. Tang
 ACM International Conference on Information & Knowledge Management (CIKM), 2023
- Accurately modeling biased random walks on weighted networks using node2vec+
 R. Liu*, M.J. Hirn, A. Krishnan
 Bioinformatics, 2023

- PyGenePlexus: A Python package for gene discovery using network-based machine learning C.A. Mancuso*, R. Liu, A. Krishnan Bioinformatics, 2023
- Taxonomy of Benchmarks in Graph Representation Learning
 R. Liu*, S. Cantürk*, F. Wnkel, S. McGuire, X. Wang, A. Little, L. O'Bray, M. Perlmutter, B. Rieck, M.J. Hirn, G. Wolf, L. Rampášek
 Learning on Graph (LoG) Conference, 2022
- GenePlexus: A web-server for gene discovery using network-based machine learning C.A. Mancuso*, P.S. Bills, D. Krum, J. Newsted, R. Liu, A. Krishnan Nucleic Acids Research, 2022
- Applications of an Association Activity Coefficient Model, NRTL-PA, to Alcohol-Containing Mixtures

A.M. Bala*, **R. Liu**, L. Peereboom, C.T. Lira Industrial & Engineering Chemistry Research, 2022

- PecanPy: a fast, efficient and parallelized Python implementation of node2vec
 R. Liu*, A. Krishnan
 Bioinformatics, 2021
- Supervised Learning is an accurate method for network-based gene classification
 R. Liu*, C.A. Mancuso*, A. Yannakoppoulos, K.A. Johnson, A. Krishnan
 Bioinformatics, 2020

Preprints and Submissions

- A General Single-Cell Analysis Framework via Conditional Diffusion Generative Models W. Tang*, R. Liu*, H. Wen, X. Dai, J. Ding, H. Li, W. Fan, Y. Xie, J. Tang bioRxiv
- CONE: COntext Specific Network Embedding via Contextualized Graph Attention
 R. Liu*, H. Yuan*, K.A. Johnson, A. Krishnan
 Submitted to MLCB'24
- Memory-Augmented Pretraining for Single-Cell Multi-Omic Analysis
 X. Dai*, H. Wen, W. Tang, R. Liu, Y. Wu, J. Ding, W. Jin, L. Yu, Y. Xie, J. Tang Submitted to IDCM'24

• Systematic study of human diseases using graph signal processing

 Single Cells Are Spatial Tokens: Transformers for Spatial Transcriptomic Data Denoising H. Wen*, W. Tang, W. Jin, J. Ding, R. Liu, F. Shi, Y. Xie, J. Tang arXiv

PRESENTATIONS

ISCB-Rocky'22

Invited Talks • Professor Trey Ideker's lab at University of California San Diego • Professor Jian Ma's lab at Carnegie Mellon University • Learning on Graphs (LoG) local meetup at Mid-North US Oral Presentations

12/2022

	12/2022
\bullet Understanding dataset characteristics via graph diffusion $SIAM\text{-}MDS'22$	09/2022
	dings $07/2022$
\bullet Accurate network-based gene classification with ultra-fast context-specific node embed $GLBIO'21$	ddings $05/2021$
Posters	
\bullet Open Biomedical Network Benchmark: A Python Toolkit for Generating Benchma with Biomedical Networks $MLCB'23$	lkring Datasets 11/2023
• A Python Toolkit for Generating Benchmarking Datasets for Machine Learning v Networks CSHL-NetBio'23	with Biological 03/2023
\bullet Pecan Py: a fast, efficient, and parallelized Python implementation for node 2vec $ISMB'20$	07/2020
\bullet Supervised-learning is an accurate method for network-based gene classification $CoCoH'19$	08/2019
\bullet Machine learning outperforms label propagation for network-based gene classification $\textit{CSHL-NetBio'} 19$	n 03/2019
ERVICES	
Teaching	
• Teaching Assistant for CMSE 201: Introduction to Computational Modeling Lecture assistant, office hours, and grading.	2020
• Grader for CHE 804: Foundations in Chemical Engineering	2019
• Grader for CHE 321: Thermodynamics for Chemical Engineering	2019
Mentoring	
Ph.D. student at University of Colorado Anschutz Medical Campus	/2023 - Present
Ongoing Project: Leveraging ontology embeddings to enable transfer learning for general forms of the control of	e classification.
Conference & Workshop Program Chairs	
• The Web Conference 2024 Graph Foundation Model Workshop Program Chair	2024
Journal and Conference Paper Reviews	
• Machine Learning in Computational Biology (MLCB)	2024
• NeurIPS Datasets and Benchmarks Track	2024
• Transactions on Knowledge and Data Engineering (TKDE)	2023 - 2024
• Transactions on Knowledge Discovery from Data (TKDD)	2023 - 2024

• F1000 Research	2023
• Cell Systems	2022
• Nature Computational Science	2022
• Bioinformatics	2021
• eLife	2019