Yuning You

RESEARCH FOCUS

Machine learning on non-Euclidean data (e.g. graphs or point clouds) and in dynamical systems, with fundamental understanding in theory and applications to real-world problems in life sciences (in particular modeling of molecular and cellular systems).

EXPERIENCES

California Institute of <u>Technology</u>, Pasadena, California

Jul 2024 - Present

Postdoctoral Scholar in Division of Biology and Biological Engineering

Advisor: Prof. Matt Thomson

Texas A&M University, College Station, Texas

Aug 2019 - Aug 2024

Ph.D. in Electrical Engineering

Graduate Research Assistant in Department of Electrical and Computer Engineering (Part-Time)

Sep 2020 – May 2024

Advisors: Prof. Yang Shen & Prof. Zhangyang (Atlas) Wang

Xi'an Jiaotong University, Xi'an, Shaanxi

Aug 2015 – Jun 2019

B.Eng. in Information Engineering

Genentech, Inc., South San Francisco, California

May 2023 – Aug 2023

Early Clinical Development/AIML Intern in Genentech Research and Early Development

🛊 insitro, Inc., South San Francisco, California

May 2022 – Aug 2022

ML Small Molecules Intern in Department of Data Science and Machine Learning

PUBLICATIONS (Check Full List on [Google Scholar])

MLGenX'25 [link]: "Building Foundation Models to Characterize Cellular Interactions via Geometric Self-Supervised Learning on Spatial Genomics", Y. You, Z. Wang, K. Fleisher, R. Liu, M. Thomson, Machine Learning for Genomics Explorations Workshop, International Conference on Learning Representations, 2025.

AIDrugX@NeurIPS'24 [link]: "Correlational Lagrangian Schrödinger Bridge: Learning Dynamics with Population-Level Regularization", **Y. You**, R. Zhou, Y. Shen, *AI for New Drug Modalities Workshop, Conference on Neural Information Processing Systems*, 2024.

HUGO'24 [link]: "Critical Assessment of Variant Prioritization Methods for Rare Disease Diagnosis within the Rare Genomes Project", ..., **Y. You**, ..., *Human Genomics*, vol. 18(44), 2024. (Impact Factor 4.50, Outcome of <u>CAGI6 RGP</u>)

ICLR'24 [link]: "Latent 3D Graph Diffusion", Y. You, R. Zhou, J. Park, H. Xu, C. Tian, Z. Wang, Y. Shen, *International Conference on Learning Representations*, oprev., 2024. (Acceptance Rate 31.00%)

NeurIPS'23 [link]: "Graph Mixture of Experts: Learning on Large-Scale Graphs with Explicit Diversity Modeling", H. Wang, Z. Jiang, Y. You, Y. Han, G. Liu, J. Srinivasa, R. Kompella, Z. Wang, Conference on Neural Information Processing Systems, pp. 50825-50837, 2023. (Acceptance Rate 26.10%)

ICLR'23 [link]: "Graph Domain Adaptation via Theory-Grounded Spectral Regularization", Y. You, T. Chen, Z. Wang, Y. Shen, *International Conference on Learning Representations*, oprev., 2023. (Acceptance Rate 31.80%)

NeurIPS'22 [link]: "Augmentations in Hypergraph Contrastive Learning: Fabricated and Generative", T. Wei*, Y. You*, T. Chen, Y. Shen, J. He, Z. Wang, Conference on Neural Information Processing Systems, pp. 1909-1922, 2022. (*Equal Contribution, Acceptance Rate 25.60%)

Bioinformatics'22 [link]: "Cross-Modality and Self-Supervised Protein Embedding for Compound-Protein Affinity and Contact Prediction", Y. You, Y. Shen, *Bioinformatics*, vol. 38(Supplement_2), pp. 68-74, 2022. (Impact Factor 6.93, MoML'22, ECCB'22 with Acceptance Rate 17.40%, 3DSIG COSI@ISMB/ECCB'21, MLSB@NeurIPS'20)

ICLR'22 [link]: "Bayesian Modeling and Uncertainty Quantification for Learning to Optimize: What, Why, and How", Y. You, Y. Cao, T. Chen, Z. Wang, Y. Shen, *International Conference on Learning Representations*, oprev., 2022. (Acceptance Rate 32.29%)

WSDM'22 [link]: "Bringing Your Own View: Graph Contrastive Learning without Prefabricated Data Augmentations", Y. You, T. Chen, Z. Wang, Y. Shen, ACM International Conference on Web Search and Data Mining, pp. 1300-1309, 2022. (Acceptance Rate 20.22%)

ICML'21 Long Presentation [link]: "Graph Contrastive Learning Automated", Y. You, T. Chen, Y. Shen, Z. Wang, *International Conference on Machine Learning*, pp. 12121-12132, 2021. (Acceptance Rate 3.01%)

TVT'21 [link]: "Probabilistic Constructive Interference Precoding for Imperfect CSIT", G. Lyu, Y. You, A. Li, X. Liao, C. Masouros, *IEEE Transactions on Vehicular Technology*, vol. 70(4), pp. 3932-3937, 2021. (Impact Factor 5.97)

NeurIPS'20 [link]: "Graph Contrastive Learning with Augmentations", Y. You*, T. Chen*, Y. Sui, T. Chen, Z. Wang, Y. Shen, Conference on Neural Information Processing Systems, pp. 5812-5823, 2020. (*Equal Contribution, Acceptance Rate 20.09%)

ICML'20 [link]: "When Does Self-Supervision Helps Graph Convolutional Networks?", Y. You*, T. Chen*, Z. Wang, Y. Shen, *International Conference on Machine Learning*, pp. 10871-10880, 2020. (*Equal Contribution, Acceptance Rate 21.80%)

CVPR'20 [link]: "L²-GCN: Layer-Wise and Learned Efficient Training of Graph Convolutional Networks", Y. You*, T. Chen*, Z. Wang, Y. Shen, *IEEE/CVF Conference on Computer Vision and Pattern Recognition*, pp. 2127-2135, 2020. (*Equal Contribution, Acceptance Rate 22.08%)

AWARDS

Distinguished Graduate Student Award for Excellence in Research, Association of Former Students of Texas A&M University [link] Mar 2025

ECEN Quality Graduate Student Award, Department of Electrical and Computer Engineering, Texas A&M University

Apr 2023

NSF Student Travel Awards, ACM International Conference on Web Search and Data Mining

Dec 2021

/ University

Chevron Scholarship, Department of Electrical and Computer Engineering, Texas A&M University
Sep 2021

Electrical and Computer Engineering PhD Merit Fellowship, Department of Electrical and Computer Engineering, Texas A&M University

Feb 2019

TALKS

Texas A&M University, Prof. James Cai's Lab, online

Oct 2023

Genentech, Inc., Spatial Omics Journal Club, online

AstraZeneca plc, AI&A Journal Club, online

Mar 2022

University of Texas at Austin, Prof. Mingyuan Zhou's Group, online

Oct 2021

Technical University of Munich, <u>Learning on Graphs and Geometry Reading Group</u> (LoGaG), online
Aug 2021

 $\underline{\text{ISMB/ECCB'21,}} \underbrace{\text{3DSIG COSI: Structural Bioinformatics and Computational Biophysics}}_{\text{Jul 2021}}, \\ \underline{\text{online [video]}}_{\text{Jul 2021}}$

ICML'21, Session of Semisupervised and Unsupervised Learning, online [video]

Jul 2021

SERVICES

Co-Organizer of AI Bootcamp VIII on Graph Machine Learning at Caltech

Session Chair of Semisupervised and Unsupervised Learning at ICML'21

Reviewer in Conferences of ICML'21-24, NeurIPS'21-24, ICLR'22,24-25, WWW'22, LoG'22,24, ISMB/ECCB' 21,23-24, ACM-BCB'21,23,24; Journals of TPAMI'21,23, TMLR'23, TNNLS'21-23, TKDE'22, TAI'22, INS'21, PeerJ'21, NEPL'21, JCST'22,24, SIPN'22, INFFUS'23, JBS'23, CSUR'24, Nature Communications Chemistry'25