Yuning You

Postdoctoral Scholar, California Institute of Technology
Email: ynyou@caltech.edu ⋄ Homepage: yyou1996.github.io

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 Technology, 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])

Preprint'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, *bioRxiv*, 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 CAGI6 RGP)

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%)

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(supp2), 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]: "L^2-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

ECEN Quality Graduate Student Award, Texas A&M University, Department of Electrical and Computer Engineering (5 Awardees). Apr 2023

NSF Student Travel Awards, ACM International Conference on Web Search and Data Mining. Dec 2021

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

Electrical and Computer Engineering PhD Merit Fellowship, Texas A&M University, Department of Electrical and Computer Engineering. Feb 2019

TALKS

Texas A&M University, Prof. James Cai's Lab, online. Oct 2023

Genentech, Inc., Spatial Omics Journal Club, online. Aug 2023

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, Learning on Graphs and Geometry Reading Group (LoGaG), online. Aug 2021

ISMB/ECCB'21, 3DSIG COSI: Structural Bioinformatics and Computational Biophysics, online. [video] 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.