# Yuning You

Ph.D. Student at Texas A&M University

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# RESEARCH INTERESTS

Machine learning on non-Euclidean data (e.g. graphs) with limited labels and distribution shifts, with fundamental understanding in theory and challenging real-world applications to biomolecules.

## **EDUCATION**

# Texas A&M University, College Station

Aug 2019 - Present

Ph.D. Student in Electrical Engineering

Advisor: Prof. Yang Shen (Unofficial Co-Advisor: Prof. Zhangyang Wang)

Xian Jiaotong University, Xi'an

Aug 2015 - Jun 2019

Bachelor of Engineering in Information Engineering

#### SELECTED PUBLICATIONS

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. (\*equal contribution, 20.09% acceptance rate)

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

Bioinformatics'22 [link]: "Cross-Modality and Self-Supervised Protein Embedding for Compound-Protein Affinity and Contact Prediction", Y. You, Y. Shen, *Bioinformatics*. (impact factor 6.93, MoML'22, ECCB'22 with 17.40% acceptance rate, 3DSIG COSI@ISMB/ECCB'21, MLSB@NeurIPS'20)

#### PROFESSIONAL EXPERIENCES

# Early Clinical Development/AIML Intern

(Expected) May 2023 - Present

Genentech Research and Early Development (gRED), Genentech, Inc., South San Francisco

Advisor: Dr. Changlin Wan Research topic: TBD

## **ML Small Molecules Intern**

May 2022 - Aug 2022

Department of Data Science and Machine Learning, insitro, Inc., South San Francisco

Advisor: Dr. Bowen Liu & Ralph Ma

Research topic: Bioactivity signatures for small-molecules

#### Applied Scientist Intern

Jun 2021 - Aug 2021

Product Semantics Team, Amazon.com Services, Inc., Remote

Advisor: Dr. Tong Zhao

Research topic: E-commerce product network embedding

# Graduate Research Assistant

Sep 2020 - Present

Department of Electrical and Computer Engineering, Texas A&M University, College Station

Advisor: Prof. Yang Shen & (Unofficial) Prof. Zhangyang Wang

Research topics: Graph machine learning, computational drug discovery

# Woluntary Research Assistant

May 2019 - Aug 2019

Intelligence SciencE and systEm Lab (iSEE), School of Data and Computer Science, Sun Yat-Sen University, Guangzhou

Advisor: Prof. Wei-Shi Zheng

Research topics: Skeleton-based action recognition, graph convolutional networks

# **(i)** Voluntary Research Assistant

Sep 2018 - Apr 2019

State Key Laboratory for Strength and Vibration of Mechanical Structures, School of Aerospace Engineering, Xi'an Jiaotong University, Xi'an

Advisors: Dr. Gangming Lyu & Prof. Guiyan Rong

Research topics: Precoding strategies in MISO downlink transmission

#### Voluntary Research Assistant

Jul 2018 - Aug 2018

Optical+Biomedical Engineering Laboratory (OBEL), School of Electrical, Electronic & Computer Engineering, University of Western Australia, Perth

Advisors: Dr. <u>Karol Karnowski</u> & Prof. <u>Barry Cense</u>

Research topic: Optical coherence tomography

#### TALKS & SERVICES

AstraZeneca, AI&A Journal Club, online.

Mar 2022

Technical University of Munich, the Learning on Graphs and Geometry Reading Group (LoGaG), online.

Aug 2021

ISMB/ECCB'21, COSI: Structural Bioinformatics and Computational Biophysics (3DSIG), online. [video] Jul 2021

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

Jul 2021

Session chair of semisupervised and unsupervised learning at ICML'21.

Reviewer in conferences of ISMB/ECCB'21,23, ACM BCB'21, ICML'21-23, NeurIPS'21-22, ICLR'22, WWW'22, LoG'22; workshops of NeurIPS'20 SSL, WWW'21 SSL, ICML'21 SSL, WWW'22 MLoG; journals of TPAMI'21,23, INS'21, TNNLS'21-22, PeerJ'21, NEPL'21, JCST'22, SIPN'22, TKDE'22, TAI'22, TMLR'23, INFFUS'23.

#### **HONORS & AWARDS**

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

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

1st Prize in Shaanxi at Contemporary Undergraduate Mathematical Contest in Modeling, China Society for Industrial and Applied Mathematics.

Dec 2016

#### **PUBLICATIONS**

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

MLSB@NeurIPS'22 [link]: "Does Inter-Protein Contact Prediction Benefit from Multi-Modal Data and Auxiliary Tasks?", A. Talukder, R. Yin, Y. Sun, Y. Shen, Y. You, Machine Learning for Structural Biology Workshop, Conference on Neural Information Processing Systems.

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. (\*equal contribution, 25.60% acceptance rate)

Bioinformatics'22 [link]: "Cross-Modality and Self-Supervised Protein Embedding for Compound-Protein Affinity and Contact Prediction", Y. You, Y. Shen, *Bioinformatics*. (impact factor 6.93, MoML'22, ECCB'22 with 17.40% acceptance rate, 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*. (32.29% acceptance rate)

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. (20.22% acceptance rate)

ICML'21 Long Presentation [link]: "Graph Contrastive Learning Automated", Y. You, T. Chen, Y. Shen, Z. Wang, International Conference on Machine Learning. (3.01% acceptance rate)

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*. (impact factor 5.97)

KDF@AAAI'21 Oral [link]: "AR-Stock: Deep Augmented Relational Stock Prediction", T. Wei, Y. You, T. Chen, Knowledge Discovery from Unstructured Data in Financial Services Workshop, Association for the Advancement of Artificial Intelligence Conference.

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. (\*equal contribution, 20.09% acceptance rate)

ICML'20 [link]: "When Does Self-Supervision Helps Graph Convolutional Networks?", Y. You\*, T. Chen\*, Z. Wang, Y. Shen, *International Conference on Machine Learning*. (\*equal contribution, 21.80% acceptance rate)

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*. (\*equal contribution, 22.08% acceptance rate)

**IPAS'18** [link]: "An Optimization Approach of Compressive Sensing Recovery Using Split Quadratic Bregman Iteration with Smoothed  $\ell_0$  Norm", G. Yang, Y. You, Z. Lu, J. Yang, Y. Wang, *IEEE International Conference on Image Processing, Applications and Systems*.