# **Shichang Zhang**

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WORK Harvard University Cambridge, MA

EXPERIENCE Postdoctoral Fellow Aug. 2024 - Present

EDUCATION University of California, Los Angeles Los Angeles, CA

Ph.D. in Computer Science June 2024

Stanford University Stanford, CA

M.S. in Statistics Apr. 2019

University of California, Berkeley Berkeley, CA

B.A. in Statistics May 2017

Honors: Honors in Statistics, High Distinction

RESEARCH Explainable AI, Trustworthy AI, Data Attribution, Mechanistic Interpretability, Large Language Interests Models, Graph Data Mining

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HONORS AND NENLP **Outstanding Paper** 2025 Awards KDD Outstanding Reviewer (Top 10%, twice, in Aug and Feb) 2025

Amazon PhD Fellowship

J.P.Morgan Chase AI PhD Fellowship

KDD Excellence in Reviewing (Top 30 of 1551)

Snap Research Fellowship Honorable Mention

ICML Top Reviewer (Top 10%)

UCLA Graduate Division Fellowship

2023

2024

2025

2026

2027

2028

2029

2029

2020

2021

Publications Refereed Publications:

 How Post-Training Reshapes LLMs: A Mechanistic View on Knowledge, Truthfulness, Refusal, and Confidence

Hongzhe Du\*, Weikai Li\*, Min Cai, Karim Saraipour, Zimin Zhang, Himabindu Lakkaraju, Yizhou Sun, **Shichang Zhang** (\*equal contribution)

Conference on Language Modeling (COLM), (NENLP Outstanding Paper), 2025

2. Automated Molecular Concept Generation and Labeling with Large Language Models Zimin Zhang\*, Qianli Wu\*, Botao Xia\*, Fang Sun, Ziniu Hu, Yizhou Sun, **Shichang Zhang** (\*equal contribution)

International Conference on Computational Linguistics (COLING), 2025

3. An Explainable AI Approach using Graph Learning to Predict ICU Length of Stay Tianjian Guo, Indranil Bardhan, Ying Ding, **Shichang Zhang** Information Systems Research (**ISR**), 2024

- 4. Motif-driven Contrastive Learning of Graph Representations **Shichang Zhang\***, Ziniu Hu\*, Arjun Subramonian, Yizhou Sun (\*equal contribution) IEEE Transactions on Knowledge and Data Engineering (**TKDE**), 2024
- Predicting and Interpreting Energy Barriers of Metallic Glasses with Graph Neural Networks Haoyu Li\*, Shichang Zhang\*, Longwen Tang, Yizhou Sun (\*equal contribution) International Conference on Machine Learning (ICML), 2024
- PaGE-Link: Graph Neural Network Explanation for Heterogeneous Link Prediction Shichang Zhang, Jiani Zhang, Xiang Song, Soji Adeshina, Da Zheng, Christos Faloutsos, Yizhou Sun The Web Conference (WWW), 2023
- GStarX: Explaining Graph Neural Networks with Structure-Aware Cooperative Games Shichang Zhang, Yozen Liu, Neil Shah, Yizhou Sun Advances in Neural Information Processing Systems (NeurIPS), 2022
- Graph-less Neural Networks, Teach Old MLPs New Tricks via Distillation Shichang Zhang, Yozen Liu, Yizhou Sun, Neil Shah International Conference on Learning Representations (ICLR), 2022
- Weak Models Can be Good Teachers: A Case Study on Link Prediction with MLPs Zongyue Qin, Shichang Zhang, Mingxuan Ju, Tong Zhao, Neil Shah, Yizhou Sun Learning on Graphs Conference (LOG), 2025
- FUSE: Measure-Theoretic Compact Fuzzy Set Representation for Taxonomy Expansion Fred Xu, Song Jiang, Zijie Huang, Xiao Luo, **Shichang Zhang**, Yuanzhou Chen, Yizhou Sun Findings of the Association for Computational Linguistics (ACL Findings), 2024
- 11. SciBench Evaluating College-Level Scientific Problem-Solving Abilities of Large Language Models
  - Xiaoxuan Wang\*, Ziniu Hu\*, Pan Lu\*, Yanqiao Zhu\*, Jieyu Zhang, Satyen Subramaniam, Arjun R Loomba, **Shichang Zhang**, Yizhou Sun, Wei Wang (\*equal contribution) International Conference on Machine Learning (**ICML**), 2024
- Laplacian Score Benefit Adaptive Filter Selection for Graph Neural Networks Yewen Wang, Shichang Zhang, Junghoo Cho, Yizhou Sun SIAM International Conference on Data Mining (SDM), 2024
- Linkless Link Prediction via Relational Distillation
   Zhichun Guo, William Shiao, Shichang Zhang, Yozen Liu, Nitesh Chawla, Neil Shah, Tong Zhao
   International Conference on Machine Learning (ICML), 2023
- Graph Condensation for Graph Neural Networks
   Wei Jin, Lingxiao Zhao, Shichang Zhang, Yozen Liu, Jiliang Tang, Neil Shah.
   International Conference on Learning Representations (ICLR), 2022

#### **Preprints:**

- Who Gets Credit or Blame? Attributing Accountability in Modern AI Systems Shichang Zhang, Hongzhe Du, Jiaqi W. Ma, Himabindu Lakkaraju (Under PNAS Review), 2025
- Towards Unified Attribution in Explainable AI, Data-Centric AI, and Mechanistic Interpretability Shichang Zhang, Tessa Han, Usha Bhalla, Himabindu Lakkaraju (Under Nature Machine Intelligence Review), 2025

3. Generalized Group Data Attribution

Dan Ley\*, **Shichang Zhang**\*, Suraj Srinivas, Gili Rusak, Himabindu Lakkaraju (\*equal contribution)

(Under Management Science Review), 2024

4. From Indirect Object Identification to Syllogisms: Exploring Binary Mechanisms in Transformer Circuits

Karim Saraipour, **Shichang Zhang** (ORIGen@COLM), 2025

- 5. On the Retention of Edited Knowledge in Fine-Tuned Language Models Fufang Wen, **Shichang Zhang** (ORIGen@COLM), 2025
- Hierarchical Compression of Text-Rich Graphs via Large Language Models Shichang Zhang, Da Zheng, Jiani Zhang, Qi Zhu, Xiang Song, Soji Adeshina, Christos Faloutsos, George Karypis, Yizhou Sun (Preprint), 2024
- Self-Control of LLM Behaviors by Compressing Suffix Gradient into Prefix Controller Min Cai, Yuchen Zhang, Shichang Zhang, Fan Yin, Difan Zou, Yisong Yue, Ziniu Hu (MI@ICML), 2024
- 8. Parameter-Efficient Tuning Large Language Models for Graph Representation Learning Qi Zhu, Da Zheng, Xiang Song, **Shichang Zhang**, Bowen Jin, Yizhou Sun, George Karypis (Preprint), 2024
- Efficient Ensembles Improve Training Data Attribution
   Junwei Deng\*, Ting-Wei Li\*, Shichang Zhang, Jiaqi Ma (\*equal contribution)
   (DMLR@ICML), 2024
- 10. A Survey on Graph Neural Network Acceleration: Algorithms, Systems, and Customized Hardware

**Shichang Zhang**, Atefeh Sohrabizadeh, Cheng Wan, Zijie Huang, Ziniu Hu, Yewen Wang, Yingyan (Celine) Lin, Jason Cong, Yizhou Sun (Under ACM Computing Review, Major Revision), 2023

Media Coverage Unifying AI Attribution: A New Frontier in Understanding Complex Systems D ^3 Insights & Experiences

June 2025

D 3 msignis & Experiences

ChatGPT has entered the classroom: how LLMs could transform education

Nature News Feature

Nov. 2023

TEACHING EXPERIENCE **Instructor**, University of California, Los Angeles

CS97: Introduction to Data Science

Summer 2024

**Teaching Assistant**, University of California, Los Angeles

CS145: Introduction to Data Mining Fall 2020, Fall 2021 CS32: Introduction to Computer Science II Spring 2021

MENTORSHIP

Arjun Subramonian (UCLA Undergrad  $\rightarrow$  UCLA PhD) Mar. 2020 - Mar. 2021 Qianli Wu (UCLA Undergrad  $\rightarrow$  Amazon SDE) Mar. 2023 - Mar. 2024 Haoyu Li (UCLA Undergrad  $\rightarrow$  UIUC PhD) Mar. 2023 - July 2024 Gaotang Li (UMich Undergrad  $\rightarrow$  UIUC PhD) Oct. 2023 - June 2024 Botao Xia (UCLA Undergrad  $\rightarrow$  UCLA Master) Oct. 2023 - Aug. 2024

Zimin Zhang (UCLA Undergrad → UIUC Master) Min Cai (Shenzhen University Master → UAlberta PhD) Hongzhe Du (UCLA Master) Karim Saraipour (UCLA Master) Fufang Wen (Columbia Master) Weikai Li (UCLA Ph.D.) Dan Ley (Harvard Ph.D.) Ethan Ji (UCLA Master) Terry Zhou (Harvard Master)	Oct. 2023 - Present Nov. 2023 - Present Mar. 2024 - Present Apr. 2024 - Present June 2024 - Present Sept. 2024 - Present Sept. 2024 - Present June 2025 - Present Sept. 2025 - Present
How Post-Training Reshapes LLMs New England NLP Meeting	Apr 2025
Peering into The Mind of AI Seminar at Georgia Institute of Technology	Apr 2025
Interpreting AI Systems Through Features, Data, and Model Components Data Mining Seminar at Emory	Apr 2025
Explainable AI for Graph Data and More AI4LIFE Group at Harvard	Feb 2024
Graph Neural Network Explanation for Heterogeneous Link Prediction Amazon Trans.AI Research Talks International World Wide Web Conference	July 2023 May 2023
Structure-Aware Graph Neural Network Explanation AI Time NeurIPS Talk Series	Feb 2023
Graph-less Neural Networks NVIDIA GNN Reading Group	May 2022
Conference Area Chair: ACL ARR - Association for Computational Linguistics Rolling Review	2025
Conference Reviewer/Program Committee:  NeurIPS - Advances in Neural Information Processing Systems ICML - International Conference on Machine Learning ICLR - International Conference on Learning Representations KDD - ACM SIGKDD Knowledge Discovery and Data Mining AAAI - AAAI Conference on Artificial Intelligence WSDM - ACM International Web Search and Data Mining Conference CIKM - ACM Conference on Information and Knowledge Management SDM - SIAM International Conference on Data Mining LOG - Learning on Graphs Conference ICDM - IEEE International Conference on Data Mining	2021 - 2025 2022 - 2025 2024 - 2026 2020, 2023 - 2025 2023 - 2025 2023 - 2025 2022 - 2023 2024 2023 2021
	Min Cai (Shenzhen University Master → UAlberta PhD) Hongzhe Du (UCLA Master) Karim Saraipour (UCLA Master) Fufang Wen (Columbia Master) Weikai Li (UCLA Ph.D.) Dan Ley (Harvard Ph.D.) Ethan Ji (UCLA Master) Terry Zhou (Harvard Master)  How Post-Training Reshapes LLMs New England NLP Meeting  Peering into The Mind of AI Seminar at Georgia Institute of Technology  Interpreting AI Systems Through Features, Data, and Model Components Data Mining Seminar at Emory  Explainable AI for Graph Data and More AI4LIFE Group at Harvard  Graph Neural Network Explanation for Heterogeneous Link Prediction Amazon Trans.AI Research Talks International World Wide Web Conference  Structure-Aware Graph Neural Network Explanation AI Time NeurIPS Talk Series  Graph-less Neural Networks NVIDIA GNN Reading Group  Conference Area Chair: ACL ARR - Association for Computational Linguistics Rolling Review  Conference Reviewer/Program Committee: NeurIPS - Advances in Neural Information Processing Systems ICML - International Conference on Learning ICLR - International Conference on Learning Representations KDD - ACM SIGKDD Knowledge Discovery and Data Mining AAAI - AAAI Conference on Artificial Intelligence WSDM - ACM International Web Search and Data Mining Conference CIKM - ACM Conference on Information and Knowledge Management SDM - SIAM International Conference on Data Mining LOG - Learning on Graphs Conference ICDM - IEEE International Conference on Data Mining

TPAMI - IEEE Transactions on Pattern Analysis and Machine Intelligence TKDD - ACM Transactions on Knowledge Discovery from Data

TKDE - IEEE Transactions on Knowledge and Data Engineering TNNLS - IEEE Transactions on Neural Networks and Learning Systems TAI - IEEE Transactions on Artificial Intelligence Management Science

## **Workshop Organizer:**

Workshop on Regulatable Machine Learning @ NeurIPS

2024 - 2025

#### **Reading Group Organizer:**

UCLA Data Mining Reading Group

2022 - 2024

**INDUSTRY** Work EXPERIENCE

SKILLS

### Amazon Web Service (AWS)

Applied Scientist Intern, Graph Machine Learning Team

Santa Clara, CA June 2023 - Nov. 2023

- Proposed a framework for applying LLMs to text-rich graph data with hierarchical neighborhood compression, which allows LLMs to leverage the graph structure and handle long input text features gathered in a rich neighborhood.
- The proposed method outperformed traditional graph ML models on node classification benchmarks and will be incorporated into the Amazon DGL project.

#### **Amazon Web Service (AWS)**

Santa Clara, CA

Applied Scientist Intern, Graph Machine Learning Team

June 2022 - Oct. 2022

- Proposed a new framework to explain GNN link prediction for recommendation on graph data, which improves user trust in the model and helps developers debug the model. Work published in WWW 2023.
- The implemented framework will be incorporated into the Amazon Neptune ML project in production.

**Snap Research** Research Intern, Computational Social Science Team

Los Angeles, CA June 2021 - Sept. 2021

- Proposed a cross-model distillation framework to transfer knowledge from GNNs to MLPs, which speeds up model inference by 179 times and facilitates model deployment on latencyconstraint applications. Work published in ICLR 2022.
- Worked on condensing large-scale training graphs to small synthetic graphs by over 90% reduction rate while maintaining competitive model performance for GNNs trained from scratch, which significantly saves storage space and achieves efficient continual learning. Work published in ICLR 2022.

WeWork Inc. Palo Alto, CA

Data Scientist Intern, Research and Applied Science Team

June 2019 - Sept. 2019

- Implemented a data processing pipeline in SQL and Python for data querying, data cleaning, and feature engineering.
- Trained a Gradient Boosted Tree model on two million customer data to predict occupancy rate for WeWork buildings and achieved 0.093 MAE on the test set.
- Presented the pricing model as a selected outstanding project to the Research and Applied Science team including the VP.

Programming: Python (PyTorch, Hugging Face, DGL), C++, R, Java, Linux, Git

Natural Languages: Mandarin Chinese (Native), English (Proficient)