

Jiayi (Raina) Xin

PHD STUDENT · COMPUTER & INFORMATION SCIENCE · SHE/HER

University of Pennsylvania, Amy Gutmann Hall, 3317 Chestnut St, Philadelphia, PA 19104

☎ +1 445-239-5869 | ✉ jiyixin@engineering.upenn.edu | 🏠 raina-xin.github.io | 🎓 Google Scholar

Education

University of Pennsylvania

Philadelphia, PA

PH.D. IN COMPUTER & INFORMATION SCIENCE (GPA 4.0/4.0)

Aug 2024 – May 2029 (Expected)

- Research Interests: LLM and Agent Evaluation; Multimodal Machine Learning; Longitudinal EHR Modeling
- Advisors: Prof. Qi Long, Prof. Weijie Su

University of Pennsylvania

Philadelphia, PA

M.SC. IN COMPUTER & INFORMATION SCIENCE (GPA 4.0/4.0)

Aug 2024 – Aug 2026

- Earned en route to the Ph.D.

The University of Hong Kong

Hong Kong

B.A.SC. IN APPLIED ARTIFICIAL INTELLIGENCE (GPA 4.06/4.30)

Sep 2020 – Jul 2024

- First Class Honours | Minor in Economics
- Undergraduate Capstone Project Mentor: Prof. Lequan Yu

Wellesley College & Massachusetts Institute of Technology

Wellesley & Cambridge, MA

UNDERGRADUATE EXCHANGE STUDENT (GPA 4.0/4.0)

Sep 2022 – Jan 2023

- MIT Undergraduate Research Opportunities Program Mentor: Prof. Connor W. Coley

Exeter College, University of Oxford

Oxford, UK

SIX-WEEK SUMMER PROGRAMME (Grade A)

Jun 2022 – Aug 2022

- Undergraduate Research Placement Mentor: Prof. David A. Clifton

Professional Experience

Microsoft

Redmond, WA

RESEARCH INTERN

May 2026 – Aug 2026

- Developed machine learning methods for biological response modeling across heterogeneous experimental contexts
- Studied how data composition affects model generalization and the design of follow-up experiments
- Host: Paidamoyo Chapfuwa

BigHat Biosciences

San Mateo, CA

MACHINE LEARNING INTERN

May 2025 – Aug 2025

- Formulated antibody reformatting as a multimodal ML problem using sequence, structure, and biophysical representations
- Developed models that generalized to previously unseen antibody families and prioritization for wet-lab follow-up
- Hosts: Hunter Elliott, Aniruddh Raghu

Goldman Sachs

Hong Kong

SUMMER ANALYST (ENGINEERING)

Jun 2023 – Aug 2023

- Built from scratch a React-based dashboard for monitoring ETL pipelines of a flagship real estate fund
- Improved operational efficiency by streamlining daily monitoring through a robust, user-friendly interface

Massachusetts Institute of Technology

Cambridge, MA

UNDERGRADUATE RESEARCHER

Sep 2022 – Jan 2023

- Gained domain expertise in untargeted tandem mass spectrometry via self-directed study and collaboration
- Prototyped the first transformer-based model for de novo chemical formula prediction from spectral data

Centaline Data Technology

Hong Kong

DATA ANALYST INTERN

Jun 2021 – Jul 2021

- Conducted data-driven market trend analysis for Hong Kong's second-hand real estate market
- Extracted insights from large-scale transaction data with both internal database and public historical data

Publications

PUBLISHED (* equal contribution)

- [P1] **Xin, J.**; Qiang, E.; Zhu, Z.; Li, X.; Su, W. J.; Long, Q. *Conformal Prediction with Paraphrase-Aware Scoring for LLM Uncertainty Quantification*. **NeurIPS 2026**, poster.
- [P2] Sun, K. *; Zhao, Y. *; **Xin, J.**; Long, Q.; Su, W. J. *CurveRL: Principled Distribution-Aware Context Reweighting for LLM Reasoning*. **NeurIPS 2026**, poster.
- [P3] Tang, Y. H. *; Yang, P. *; **Xin, J.** *; Shang, T.; Chen, X.; Yuan, Y.; Lian, Y.; Long, Q. *TrialDesignBench: Benchmarking Language Models for Phase-I Trial Design Against Clinical Knowledge*. **NeurIPS 2026 Workshop on World Models for Health and Science**, poster.
- [P4] **Xin, J.**; Li, X.; Qiang, E.; He, W.; Shang, T.; Su, W. J.; Long, Q. *UCS: Estimating Unseen Coverage for Improved In-Context Learning*. **ACL 2026 Findings**.
- [P5] Ballard, J.; **Xin, J.**; Beeche, C.; Sharma, R.; Zhao, X.; Zhang, R.; Dong, J.; Shen, L.; Chen, T.; Witschey, W.; Long, Q. *An Interpretable Multimodal Framework for Calibrated Cardiovascular Disease Risk Prediction Leveraging Heterogeneous EHR and Imaging Data*. **AMIA 2026 Annual Symposium**, accepted.
- [P6] Zhang, R. *; Dong, J. *; **Xin, J.**; Ballard, J.; Beeche, C.; Sharma, R.; Zhao, X.; Konz, N.; Long, Q.; Witschey, W.; Chen, T. *CURA: Calibrated Uncertainty with Retrieval and Agents for Trustworthy Multimodal Medical Decision Support*. **MICCAI 2026**, accepted.
- [P7] Sharma, R.; Beeche, C.; Dong, N.; Qu, H.; Zhuang, R.; Zhang, R.; Gangaram, V.; Goswami, P.; **Xin, J.**; Ballard, J.; Zhang, G.; Goldberg, A.; Sagreiya, H.; Long, Q.; Chen, T.; Witschey, W. *DISCERN: A Clinical Impact-aware Framework for Radiology Report Comparison*. **AMIA 2026 Annual Symposium**, accepted.
- [P8] **Xin, J.**; Yun, S.; Peng, J.; Choi, I.; Ballard, J. L.; Chen, T.; Long, Q. *I²MoE: Interpretable Multimodal Interaction-aware Mixture-of-Experts*. **ICML 2025**, poster.
- [P9] **Xin, J.**; Raghu, A.; Bhattacharya, N.; Carr, A.; Montgomery, M.; Elliott, H. *Improved Therapeutic Antibody Reformating through Multimodal Machine Learning*. **NeurIPS 2025 AI4Science and FM4LS Workshops**, poster.
- [P10] Yun, S. *; **Xin, J.** *; Choi, I.; Peng, J.; Ding, Y.; Long, Q.; Chen, T. *Generate, Then Retrieve: Addressing Missing Modalities in Multimodal Learning via Generative AI and MoE*. **AAAI 2025 GenAI4Health Workshop**. 🏆 **Best Paper Award**.
- [P11] Wang, F.; **Xin, J.**; Zhao, W.; Jiang, Y.; Yeung, M.; Wang, L.; Yu, L. *TAD-Graph: Enhancing Whole Slide Image Analysis via Task-Aware Subgraph Disentanglement*. **IEEE Transactions on Medical Imaging**, 44(6): 2683–2695 (2025).
- [P12] Li, Y.; **Xin, J.**; Miao, M. M.; Long, Q.; Ungar, L. *The Impact of Language Mixing on Bilingual LLM Reasoning*. **EMNLP 2025**. 🏆 **Oral**.
- [P13] Peng, J.; Ballard, J. L.; Zhang, M.; Yun, S.; **Xin, J.**; Long, Q.; Zhang, Y.; Chen, T. *Modalities Contribute Unequally: Enhancing Medical Multi-modal Learning through Adaptive Modality Token Re-balancing*. **ICML 2025**, poster.
- [P14] Goldman, S. *; **Xin, J.** *; Provenzano, J.; Coley, C. W. *MIST-CF: Chemical Formula Inference from Tandem Mass Spectra*. **Journal of Chemical Information and Modeling**, 64(7): 2421–2431 (2024).
- [P15] Ma, C.; Zhao, H.; Zheng, L.; **Xin, J.**; Li, Q.; Wu, L.; Deng, Z.; Lu, Y. Y.; Liu, Q.; Wang, S.; Kong, L. *Retrieved Sequence Augmentation for Protein Representation Learning*. **EMNLP 2024**, poster.
- [P16] Yun, S.; Choi, I.; Peng, J.; Wu, Y.; Bao, J.; Zhang, Q.; **Xin, J.**; Long, Q.; Chen, T. *Flex-MoE: Modeling Arbitrary Modality Combination via the Flexible Mixture-of-Experts*. **NeurIPS 2024**. 🏆 **Spotlight**.
- [P17] Goldman, S.; Bradshaw, J.; **Xin, J.**; Coley, C. W. *Prefix-Tree Decoding for Predicting Mass Spectra from Molecules*. **NeurIPS 2023**. 🏆 **Spotlight**.
- [P18] Su, H.; Kasai, J.; Wu, C. H.; Shi, W.; Wang, T.; **Xin, J.**; Zhang, R.; Ostendorf, M.; Zettlemoyer, L.; Smith, N. A.; Yu, T. *Selective Annotation Makes Language Models Better Few-Shot Learners*. **ICLR 2023**, poster.
- [P19] Ma, S.; Yee, C.-Y.; **Xin, J.**; Ho, J. W. K. *AI Clinical Applications of Wearable Technologies*. In **Wearable Technology in Medicine and Health Care**. IOP Publishing (2023).

REVISED AND RESUBMITTED

- [R1] Li, X.; **Xin, J.**; Long, Q.; Su, W. J. *Evaluating the Unseen Capabilities: How Many Theorems Do LLMs Know?* arXiv:2506.02058 (2025). Revise and resubmit to **Proceedings of the National Academy of Sciences (PNAS)**.
- [R2] Yun, S.; **Xin, J.**; Choi, I.; Peng, J.; Ding, Y.; Long, Q.; Chen, T. *Mixture-of-Experts for Multimodal Learning with Missing Modalities*. Revise and resubmit to **IEEE Transactions on Pattern Analysis and Machine Intelligence (TPAMI)**.
- [R3] Choi, I.; Yun, S.; **Xin, J.**; Peng, J.; Chen, T.; Long, Q. *M2G-LLM Enhancing Clinical Prediction via Multimodal Graph Reasoning and LLM Context Injection*. Revise and resubmit to **npj Artificial Intelligence**.

UNDER REVIEW

- [U1] **Xin, J.**; Shang, T.; Choi, I.; Sun, K.; Park, Y.-H.; Gu, J.; Long, Q. *REAL-EHR: Benchmarking Long-Horizon Clinical Event Forecasting*. Submitted to **ICLR 2027**.
- [U2] **Xin, J.**; Shang, T.; Qiang, E.; Tan, Z.; Ke, S.; Chen, T.; Long, Q. *TRACE: Trajectory-Aware Residual Correction for Longitudinal EHR Prediction*. Submitted to **ACL ARR 2026 Oct**.
- [U3] **Xin, J.**; Shang, T.; Choi, I.; Sun, K.; Park, Y.-H.; Gu, J.; Long, Q. *Belief-State World Models for Longitudinal EHR Forecasting*. Submitted to **ACL ARR 2026 May**.
- [U4] Lian, Y.; **Xin, J.**; Mishra-Kalyani, P.; Yuan, Y.; Meric-Bernstam, F.; Parikh, R.; Sallée, V.; Vonderheide, R. H.; Long, Q. *Reimagining Clinical Trials in the Era of Generative AI: Toward Lifecycle-Integrated, Agentic Systems*. Revise and resubmit to **Communications Medicine**.

Awards, Fellowships, & Grants

2026	🏆 IMC PhD Fellowship Finalist, IMC Trading (one of seven finalists)	\$5,000
2025	PhD Career Exploration Fellowship, Penn (hosted by Amazon AWS Security 🔗)	
2024	Graduate Fellowship and Research Stipend Award, Penn Engineering Dean's Honours List, HKU Faculty of Science (top 10% of class)	\$40,000
2023	🏆 Winnie S M Tang Scholarship in Applied AI, HKU (sole junior recipient) C.V. Starr Scholarships, HKU Dean's Honours List, HKU Faculty of Science (top 10% of class)	HKD 20,000 HKD 5,000
2022	🏆 Winnie S M Tang Scholarship in Applied AI, HKU (sole sophomore recipient) Worldwide Undergraduate Student Exchange Scholarships, HKU Talent Development Scholarship, HKSAR Government Scholarship Fund	HKD 20,000 HKD 5,000 HKD 5,000
2021	🏆 Laidlaw Research and Leadership Scholarship 🔗 , Laidlaw Foundation Dean's Honours List, HKU Faculty of Science (top 10% of class)	HKD 10,000
2020	Future Leaders of the Year Scholarship, HKU	HKD 20,000

Presentations

* equal contribution; + presenting author

- [T1] **Xin, J.**⁺; Li, X.; Qiang, E.; He, W.; Shang, T.; Su, W. J.; Long, Q. *UCS: Estimating Unseen Coverage for Improved In-Context Learning*. Poster, **AWS ASSET Trustworthy AI Symposium**, Philadelphia, PA, 2026.
- [T2] **Xin, J.**⁺; Li, X.; Qiang, E.; He, W.; Shang, T.; Su, W. J.; Long, Q. *UCS: Estimating Unseen Coverage for Improved In-Context Learning*. Poster, **ACL Annual Meeting**, San Diego, CA, 2026.
- [T3] **Xin, J.**⁺; Qiang, E.; Zhu, Z.; Li, X.; Su, W. J.; Long, Q. *Conformal Prediction with Paraphrase-Aware Scoring for LLM Uncertainty Quantification*. 🎤 **Oral presentation, NISS Virtual New Researchers Conference**, 2026.
- [T4] **Xin, J.**⁺. *Reliable Agentic AI under Partial Evidence and Regime Shift*. 🗣️ **Invited presentation, IMC Trading PhD Fellowship Research Connect Event**, Chicago, IL, 2026.

- [T5] **Xin, J.**⁺; Yun, S.; Peng, J.; Choi, I.; Ballard, J. L.; Chen, T.; Long, Q. *I²MoE: Interpretable Multimodal Interaction-aware Mixture-of-Experts*. Poster, **AASF AIX Summit**, New York, NY, 2026.
- [T6] Li, X.; **Xin, J.**⁺; Long, Q.; Su, W. J. *Evaluating the Unseen Capabilities: How Many Theorems Do LLMs Know?* 📺 **Invited presentation, ENAR Spring Meeting**, Indianapolis, IN, 2026.
- [T7] **Xin, J.**⁺; Raghu, A.; Bhattacharya, N.; Carr, A.; Montgomery, M.; Elliott, H. *Improved Therapeutic Antibody Reformating through Multimodal Machine Learning*. Poster, **NeurIPS AI4Science and FM4LS Workshop**, San Diego, CA, 2025.
- [T8] **Xin, J.**⁺; Yun, S.; Peng, J.; Choi, I.; Ballard, J. L.; Chen, T.; Long, Q. *I²MoE: Interpretable Multimodal Interaction-aware Mixture-of-Experts*. Poster, **Penn DBEI Big Data Conference**, Philadelphia, PA, 2025.
- [T9] **Xin, J.**⁺; Yun, S.; Peng, J.; Choi, I.; Ballard, J. L.; Chen, T.; Long, Q. *I²MoE: Interpretable Multimodal Interaction-aware Mixture-of-Experts*. Poster, **Penn Engineering AI Research Mixer**, Philadelphia, PA, 2025.
- [T10] Yun, S. *; **Xin, J.** **; Choi, I.; Peng, J.; Ding, Y.; Long, Q.; Chen, T. *Generate, Then Retrieve: Addressing Missing Modalities in Multimodal Learning via Generative AI and MoE*. 🗣️ **Oral presentation, AAAI GenAI4Health Workshop**, Philadelphia, PA, 2025.

Teaching Practicum

- 2026 **CETLI University Teaching Certificate**, Penn Center for Excellence in Teaching, Learning and Innovation (CETLI)
- 2026 **CIS 5190 Applied Machine Learning**, Teaching Assistant
- 2025 **CIS 5190 Applied Machine Learning**, Teaching Assistant
- 2024 **Onsite TA Training and Workshops**, UPenn CETLI

Outreach & Professional Development

SERVICE AND OUTREACH

- 2025 **CIS 4190/5190 Applied Machine Learning**, Guest Lecturer on NLP Module 2
- 2025 **Penn AI Inside the Research Series**, Featured Speaker 📺 **Video**
- 2024 **UPenn Intercultural Leadership Program**, Participant
- 2024 **HKU Faculty of Science**, Invited Speaker, Alumni Sharing 📺 **Video**
- 2023–2024 **HKU Faculty of Science**, Student Peer Advisor (🏆 **Outstanding SPA, one of five**)
- 2023–2024 **HKU Artificial Intelligence & Data Literacy Student Interest Group**, Person in Charge
- 2022 **Make_Sense Mexico**, Community Influencer
- 2021 **HKU Faculty of Science**, Invited Speaker, Student Sharing 📺 **Video**

PEER REVIEW

- **Journals:** IEEE Transactions on Multimedia (2026), Medical Image Analysis (2026), Array (2026), Expert Systems With Applications (2026)
- **Conferences:** NeurIPS (2025, 2026), ICML (2025, 2026), ICLR (2026, 2027), AAAI (2026, 2027), ACL ARR (2026 Jan, 2026 May, 2026 Aug), MICCAI (2026), ACM BCB (2026), AMIA (2026)
- **Workshops:** SCOPE (ICLR 2025), AI4Science (NeurIPS 2026, ICML 2026), FM4LS (ICML 2026), LASS (CIKM 2026)

PROFESSIONAL MEMBERSHIPS

- Student Member: Association for Computational Linguistics (ACL)
- Student Member: International Biometric Society, Eastern North American Region (ENAR)
- CFA® Program Candidate, Level II: Affiliated with CFA Society Philadelphia