Lanqing Li

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Personal Profile

- I'm a principal investigator at Zhejiang Lab starting from Jan 2023, leading the computational genomics group at the Research Center for Computational Life Sciences. Previously I was a senior research scientist (T10) at Tencent AI Lab, working on machine learning and its applications in drug discovery and autonomous control. I also worked as a tech lead at InferVision, a pre-IPO medical AI startup.
- **Homepage**: https://lanqingli1993.github.io/
- **Research Interests**: Machine Learning, Reinforcement Learning (RL), AI for Drug Discovery (AIDD), AI for Science.
- **Research Highlights**: As a machine learning researcher, I pioneered a new reinforcement learning paradigm called offline meta-RL (OMRL) for pre-training powerful decision-making models and AI agents, by inventing one of the first model-free OMRL algorithms FOCAL. I subsequently proposed a theoretical framework called UNICORN to unify existing works in the field, providing principled guidelines for future research.

Employment History

Zhejiang Lab *Hangzhou, China*

Principal Investigator, Research Center for Computational Life Sciences *01/2023-Now*

- R&D of RL-based and LLM-based AI agent for drug discovery and biomolecular design.
- Leading several core AIDD projects:
  1. Design of virus-like particle (VLP)-based delivery system.
  2. Synthesis planning and biocatalysis modeling.
  3. mRNA vaccine and sequence design.
- Mentor of 4 employees and 10+ Ph.D. students.

Shenzhen Tencent Computer System Co., Ltd. *Shenzhen, China*

Senior Research Scientist, AI Lab *10/2019-01/2023*

- Co-developed the multi-step retrosynthesis module of iDrug. Independently developed a state-of-the-art model for synthetic accessibility prediction, in collaboration with the American Chemical Society (CAS).
- Led the research and development of the core AI algorithms and greenhouse simulator of the iGrow solution, in collaboration with Wageningen University & Research (WUR).
- Co-mentored the Tencent AI Lab Rhino-Bird Elite Training Program and Tencent AI Lab Rhino-Bird Focused Research Program, with focuses on robust learning and retrosynthesis.
- Mentor of 1 employee and 20+ interns at the machine learning center.

Infervision Medical Technology Co., Ltd. *Beijing, China*

Tech Lead & Machine Learning Engineer *03/2018-10/2019*

- Led a team of 8 engineers to develop computer-aided detection (CAD) solutions like InferRead Mammo Breat and InferRead CT Coronary.

Academic History

The Chinese University of Hong Kong *08/2022-Now*

Ph.D. Candidate in Computer Science and Engineering

- Supervisor: Prof. Pheng Ann Heng
- Research area: Robust Learning, AI for Science

The University of Chicago *09/2015-2017/08*

Master of Science (Ph.D. Program) in Physics

- Concentration: Theoretical Biophysics & Computer Vision

Massachusetts Institute of Technology *08/2012-06/2015*

Bachelor of Science in Physics *Major GPA: 4.7/5.0*

- Advised by Prof. Alan Guth, Prof. David Kaiser and Prof. Nevin Weinberg.
- Concentration: Theoretical Cosmology, High Energy Physics

Imperial College London *06/2014-08/2014*

Exchange Student of Summer Research Placement

Peking University *09/2011-06/2012*

Candidate for a Bachelor of Science in Physics *Major GPA: 3.88/4.0*

Selected Publications (*: co-first author, †: corresponding author)

- **Articles in Peer-Reviewed Journals**
  1. Ma, K., Yang, H., Yang, S., Zhao, K., **Li, L.**, Chen, Y., Huang, J., Cheng, J., Rong, Y. "Solving the non-submodular network collapse problems via Decision Transformer." Neural Networks (2024): 106328.
  2. Liu, Z., Liu, L., Wu, B., **Li, L.**, Wang, X., Yuan, B., Zhao, P. Dynamics Adapted Imitation Learning. Transactions on Machine Learning Research (2023).
  3. Gao, Z., Jiang, C., Zhang, J., Jiang, X., **Li, L.**, Zhao, P., Yang, H., Huang, Y., Li, J. *Hierarchical graph learning for protein–protein interaction*. Nature Communications 14.1 (2023): 1093.
- **Articles in Peer-Reviewed Conference Proceedings**
  1. **Li, L.***, Zhang, H.*, Zhang, X., Zhu, S., Yu, Y., Zhao, J., Heng, P. Towards an Information Theoretic Framework of Context-based Offline Meta-Reinforcement Learning. NeurIPS 2024 **Spotlight**.
  2. Zhou, Z.*, **Li, L.***, Zhao, P., Heng, P., Gong, W. Class-Conditional Sharpness-Aware Minimization for Deep Long-Tailed Recognition. CVPR 2023.
  3. Wang, D., **Li, L.**†, Zhao, P., Heng, P., Zhang, M. On the Pitfall of Mixup Training for Uncertainty Calibration. CVPR 2023.
  4. Zeng, L., **Li, L.**†, Gao, Z., Zhao, P., Li, J. ImGCL: Revisiting Graph Contrastive Learning on Imbalanced Node Classification. AAAI 2023.
  5. Gao, Z., Niu, Y., Cheng, J., Tang, J., Xu, T., Zhao, P., **Li, L.**†, Tsung, F., Li, J. Handling Missing Data via Max-Entropy Regularized Graph Autoencoder. AAAI 2023.
  6. Liu, S., Ying, R., Dong, H., **Li, L.**†, Xu, T., Rong, Y., Zhao, P., Huang, J., Wu, D. Local Augmentation for Graph Neural Networks. ICML 2022.
  7. **Li, L.**, Yang, R., Luo, D. FOCAL: Efficient Fully-Offline Meta-Reinforcement Learning via Distance Metric Learning and Behavior Regularization. ICLR 2021.
- **In Submission to Journals and Conferences**
  1. **Li, L.***, Zeng, L.*, Gao, Z., Yuan, S., Bian, Y., Wu, B., Zhou, Z., Xu, H., Li, J., Zhao, P., Heng, P. Benchmarking Imbalanced Learning for AI-Aided Drug Discovery. Under major revision by Nature Communications.
  2. Huang, Y.*, **Li, L.***, Qian, W., Yu, J., Zhao, H., Zhang, O., Chen, G., Gu, S., Heng, P., Hou, T., Kang, Y. ERAM: A Unified Dual-Grained Cross-Modal Molecular Representation Learning Framework for Enzymatic Reaction. Under review by Advanced Science.
  3. Zhang, H., Zheng, B., Ji, T., Liu, J., Guo, A., Zhao, J.†, **Li, L.**†. Scrutinize What We Ignore: Reining In Task Representation Shift Of Context-Based Offline Meta Reinforcement Learning. Under review by ICLR 2025. (current scores: 6, 6, 8, 8)

Selected Awards

NSFC Young Scientists Fund *2024*

Prize of Sustainable Social Values, Tencent *2021*

SAIL Award at World Artificial Intelligence Conference - Finalist *2020*

Distinguished Sachs Fellowship, UChicago *2015*

Li & Fung Scholarship, MIT *2014*

Jay Tsun Shaw (1946) Memorial Scholarship, MIT *2013-2015*

First Prize in Young Physicists Tournaments, Peking University *2012*

Mingde Scholarship, Peking University *2011*

Excellent Student Scholarship, Peking University *2011*

Gold Medalist of International Physics Olympiad *2011*

- *Ranked 1st in Theory and 5th in Total Score*
- *Prize of Best Score in Theory (Full Marks)*

Academic Activities

- **Invited Talks and Seminars**
  1. *AI Agent: Principles and Applications*, 1st speaker at CAAI Embodied AI Youth Symposium, invited by Prof. Junqiao Zhao. (12/2023)
  2. *Intelligent Drug Discovery Platform and Its Applications*, presented at the "Computation + Biology" Youth Academic Research Symposium, Zhejiang lab. (09/2023)
  3. *Guest lecture on reinforcement learning applications*, The Chinese University of Hong Kong, Shenzhen, invited by Prof. Baoxiang Wang. (02/2023)
- **Services**
  - Area Chair, ICML 2025
  - Reviewer, TPAMI
  - Reviewer, ICLR 2024
  - Reviewer, CVPR 2023
  - Reviewer, ICML 2022, 2023
  - Reviewer, NeurIPS 2022, 2023
  - Reviewer, IJCAI 2021, 2022
- **Teaching and Mentoring**
  1. TA of PHYS 130 Series, UChicago *09/2016-06/2017*
  2. TA of PHYS 14200 Honors Electricity & Magnetism, UChicago *01/2016-03/2016*
  3. TA of PHYS 14100 Honors Mechanics, UChicago *09/2015-12/2015*
  4. PRIMES Circle Mentor, MIT Department of Mathematics *02/2014-12/2014*
- **Science Outreach**
  - *Modeling Biological World with Intelligent Computing*, interview by Zhejiang Lab. (11/2023)
  - *Artificial Protein Design with Inverse Folding Models*, interview by CCTV-3. (09/2023)