# Yang Lu

# Curriculum Vitae

# RESEARCH INTERESTS

# 1 Machine Learning.

- o Interpretable machine learning
- Error-controlled machine learning
- Al for science/healthcare

#### 2 Computational Biology and Bioinformatics.

- Computational genomics/proteomics/microbiomics
- Multi-omics integration
- Agents for Bioinformatics analysis

# **EDUCATION**

#### 2017 Ph.D. in Computational Biology and Bioinformatics.

University of Southern California, Los Angeles, CA, USA

Thesis: "Big Data Analytics in Metagenomics: Integration, Representation, Management, and

Visualization".

Advisor: Dr. Fengzhu Sun

#### 2013 M.S. in Computer Science and Engineering.

Shanghai Jiao Tong University, Shanghai, China

## 2010 B.S. in Computer and Software Engineering.

Shanghai Jiao Tong University, Shanghai, China

# PROFESSIONAL APPOINTMENTS

08/2025-	University of	Wisconsin-N	/ladison,	Madison,	WI, I	USA.
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- Assistant Professor of Biomedical Engineering
- Assistant Professor of Biostatistics & Medical Informatics
- 02/2025- ByteDance Seed, Seattle, WA, USA.
  - Visiting Research Scientist
- 01/2023- University of Waterloo, Waterloo, Ontario, Canada.
- 07/2025 Assistant Professor of Computer Science
- 01/2018- University of Washington, Seattle, WA, USA.
- 11/2022 Postdoctoral Fellow at Department of Genome Sciences
  - o Advisor: Dr. William S. Noble
- 09/2015– University of Southern California, Los Angeles, CA, USA.
- 08/2017 Research Assistant at Department of Quantitative and Computational Biology
  - o Advisor: Dr. Fengzhu Sun
- 06/2011- Microsoft Research Asia, Beijing, China.
- 11/2011 Research Intern

11/2010- Microsoft Azure, Shanghai, China.

05/2011 • Software Engineer Intern

04/2010- **Tencent Research**, Shanghai, China.

08/2010 • Software Engineer Intern

# PUBLICATIONS

\* indicates equal contribution. † indicates the corresponding author.

#### PUBLICATIONS AS LEADING OR CORRESPONDING AUTHOR

- 1. Z Dong, H Zhou, Y Jiang, V Zhong, and  $\underline{YY Lu}^{\dagger}$ . "Simplifying bioinformatics data analysis through conversation". bioRxiv:10.1101/2023.10.29.564479, 2024.
- 2. H Zhou, K Cao, and YY Lu<sup>†</sup>. "Securing diagonal integration of multimodal single-cell data against ambiguous mapping". **Bioinformatics**, In press, 2025.
- 3. W Chen, Y Jiang, WS Noble, and  $\underline{YY Lu}^{\dagger}$ . "Error-controlled non-additive interaction discovery in machine learning models". **Nature Machine Intelligence**, In press, 2025.
- 4. Y Jiang, M Aton, Q Zhu<sup>†</sup>, and <u>YY Lu</u><sup>†</sup>. "Modeling microbiome-trait associations with taxonomy-adaptive neural networks". **Microbiome**, 13(87), 2025.
- 5. Y Jiang, D Liao, Q Zhu, and YY Lu<sup>†</sup>. "PhyloMix: Enhancing microbiome-trait association prediction through phylogeny-mixing augmentation". **Bioinformatics**, 41(2):btaf014, 2025.
- 6. <u>YY Lu</u>, WS Noble, and U Keich. "A BLAST from the past: revisiting BLAST's E-value". **Bioinformatics**, 40(12):btae729, 2024.
- 7. W Chen, WS Noble<sup>†</sup>, and YY Lu<sup>†</sup>. "DeepROCK: Error-controlled interaction detection in deep neural networks". **NeurIPS Intepretable AI Workshop**, 2024.
- 8. Z Ma\*, YY Lu\*†, Y Wang, R Lin, Z Yang, F Zhang, and Y Wang†. "Metric Learning for Comparing Genomic Data with Triplet Network". **Briefings in Bioinformatics**, 23(5):bbac345, 2022.
- 9. <u>YY Lu</u> and WS Noble. "A wider field of view to predict expression". **Nature Methods**, 18:1155-1156, 2021.
- 10. <u>YY Lu</u>\*, W Guo\*, X Xing, and WS Noble. "DANCE: Enhancing saliency maps using decoys". International Conference on Machine Learning (**ICML**), 2021.
- 11. YY Lu, T Yu, G Bonora, and WS Noble. "ACE: Explaining cluster from an adversarial perspective". International Conference on Machine Learning (ICML), 2021.
- 12. <u>YY Lu</u>, J Bilmes, RA Rodriguez-Mias, J Villen, and WS Noble. "DIAmeter: Matching peptides to data-independent acquisition mass spectrometry data". International Conference on Intelligent Systems for Molecular Biology (**ISMB**), 2021.
- 13. YY Lu\*, J Bai\*, Y Wang, Y Wang, and F Sun. "CRAFT: Compact genome Representation towards large-scale Alignment-Free daTabase". **Bioinformatics**, 37(2):155-161, 2020.
- 14. J Schreiber\*, <u>YY Lu</u>\*, and WS Noble. "Ledidi: Designing genomic edits that induce functional activity". **ICML Workshop on CompBio**, 2020.
- 15. <u>YY Lu</u>\*, Y Fan\*, J Lv, and WS Noble. "DeepPINK: reproducible feature selection in deep neural networks". Advances in Neural Information Processing Systems (**NeurIPS**), 8676-8686, 2018
- 16. <u>YY Lu</u>. "Big Data Analytics in Metagenomics: Integration, Representation, Management, and Visualization". **Doctoral Thesis**. University of Southern California, 2017.
- 17. YY Lu, J Lv, JA Fuhrman, and F Sun. "Towards enhanced and interpretable clustering/classification in integrative genomics". **Nucleic Acids Research**, 45(20):e169, 2017.
- 18. <u>YY Lu</u>, K Tang, J Ren, JA Fuhrman, MS Waterman, and F Sun. "CAFE: aCcelerated Alignment-FrEe sequence analysis". **Nucleic Acids Research**, 45(W1):W554-W559, 2017.
- YY Lu, T Chen, JA Fuhrman, and F Sun. "COCACOLA: binning metagenomic contigs using sequence COmposition, read CoverAge, CO-alignment and paired-end read LinkAge". Bioinformatics, 33(6):791-798, 2017.

#### PUBLICATIONS AS SUPPORTING AUTHOR

- 1. J Schreiber, FK Lorbeer, M Heinzl, <u>YY Lu</u>, A Stark and WS Noble. "Programmatic design and editing of cis-regulatory elements". bioRxiv:10.1101/2025.04.22.650035, 2025.
- A Kertesz-Farkas, FLA Acquaye, V Ostapenko, RH Locon, <u>YY Lu</u>, CE Grant and WS Noble. "Fast and memory efficient searching of large-scale mass spectrometry data using Tide". bioRxiv:10.1101/2025.04.01.646675, 2025.
- 3. F Alipour, C Holmes, <u>YY Lu</u>, KA Hill and L Kari. "Leveraging machine learning for taxonomic classification of emerging astroviruses". **Frontiers in Molecular Biosciences**, 10:1305506, 2024.
- 4. C Ma, H Zhao, L Zheng, J Xin, Q Li, L Wu, Z Deng, <u>YY Lu</u>, Q Liu, and L Kong. "Retrieved Sequence Augmentation for Protein Representation Learning". Empirical Methods in Natural Language Processing (**EMNLP**), 2024.
- 5. A Kertesz-Farkas, FL Nii Adoquaye Acquaye, K Bhimani, JK Eng, WE Fondrie, C Grant, MR Hoopmann, A Lin, <u>YY Lu</u>, RL Moritz, MJ MacCoss, and WS Noble. "The Crux Toolkit for Analysis of Bottom-Up Tandem Mass Spectrometry Proteomics Data". **Journal of Proteome Research**, 22(2):561-569, 2023.
- 6. AB Dincer, <u>YY Lu</u>, D Schweppe, S Oh, and WS Noble. "Reducing peptide sequence bias in quantitative mass spectrometry data with machine learning". **Journal of Proteome Research**, 21(7):1771-1782, 2022.
- 7. Z Wang, Z Wang, YY Lu, F Sun, and S Zhu. "SolidBin: Improving Metagenome Binning with Semi-supervised Normalized Cut". **Bioinformatics**, 35(21):4229-4238, 2019.
- 8. DF Read, K Cook, <u>YY Lu</u>, KG Le Roch, and WS Noble. "Predicting gene expression in the human malaria parasite Plasmodium falciparum using histone modification, nucleosome positioning, and 3D localization features". **PLoS Computational Biology**, 15(9):e1007329, 2019.
- A Hu, <u>YY Lu</u>, J Bilmes, and WS Noble. "Joint precursor elution profile inference via regression for peptide detection in data-independent acquisition mass spectra". **Journal of Proteome Research**, 18(1):86-94, 2018
- 10. J Ren, X Bai, <u>YY Lu</u>, K Tang, Y Wang, G Reinert, and F Sun. "Alignment-free sequence analysis and applications". **Annual Review of Biomedical Data Science**, 1:93-114, 2018.
- 11. K Tang, <u>YY Lu</u>, and F Sun. "Background Adjusted Alignment-free Dissimilarity Measures Improve the Detection of Horizontal Gene Transfer". **Frontiers in Microbiology**, 9:711, 2018.
- 12. Y Wang, K Wang, YY Lu, and F Sun. "Improving contig binning of metagenomic data using  $d_2^S$  oligonucleotide frequency dissimilarity". **BMC Bioinformatics**, 18(1):425, 2018.
- 13. J Ren, NA Ahlgren, <u>YY Lu</u>, JA Fuhrman, and F Sun. "VirFinder: a novel k-mer based tool for identifying viral sequences from assembled metagenomic data". **Microbiome**, 5(1):69, 2017.
- 14. NA Ahlgren, J Ren,  $\underline{YY}$  Lu, JA Fuhrman, and F Sun. "Alignment-free  $d_2^*$  oligonucleotide frequency dissimilarity measure improves prediction of hosts from metagenomically-derived viral sequences". **Nucleic Acids Research**, 45(1):39-53, 2017.

# — GRANTS

2023 – 2028 NSERC Discovery Grant, Natural Sciences and Engineering Research Council of Canada.

• Title: Uncertainty-aware integrative pattern discovery for single-cell analysis

o Role: PI

o Amount: \$167,500

# INVITED TALKS

- 2025 International Conference on Intelligent Biology and Medicine (ICIBM)
  - Joint Conference on Statistics and Data Science in China (JCSDS)
  - o Purdue University, Department of Computer Science
  - o The Ohio State University, Department of Biomedical Informatics
  - o MidSouth Computational Biology and Bioinformatics Society (MCBIOS)
  - University of Pittsburgh, DBMI Colloquium
  - Michigan State University, Department of Computational Mathematics, Science and Engineering
  - University of Texas MD Anderson Cancer Center, Data Science and Modeling Forum
- 2024 University of Wisconsin–Madison, Department of Biomedical Engineering
  - o Cold Spring Harbor Laboratory, Biological Data Science meeting
  - Intelligent Systems for Molecular Biology (ISMB)
  - University of British Columbia, Michael Smith Laboratories
  - o University of Maryland, Department of Computer Science
- 2023 Amgen, Data Sciences
  - o Western University, Bioinformatics Seminar
  - o University of Ottawa, Technologies for Microbiome Science and Engineering seminar
- 2022 HSE University, School of Data Analysis and Artificial Intelligence
  - o University of Texas MD Anderson Cancer Center, Data Science and Modeling Forum
  - o Chinese Academy of Sciences, Academy of Mathematics and Systems Science
  - o University of Toronto, Donnelly Centre for Cellular and Biomolecular Research
  - University of Waterloo, Cheriton School of Computer Science
  - University of Oregon, Department of Computer and Information Science
  - Georgia Institute of Technology, School of Computational Science and Engineering
  - University of Notre Dame, Department of Computer Science and Engineering
  - University of Texas MD Anderson Cancer Center, Department of Bioinformatics and Computational Biology
  - o Pennsylvania State University, Department of Computer Science and Engineering
  - University of Washington, Paul G. Allen School of Computer Science and Engineering
  - o Drexel University, College of Computing and Informatics
  - National University of Singapore, Department of Biological Sciences
  - o Indiana University School of Medicine, Herman B Wells Center for Pediatric Research
  - University of Florida, Department of Health Outcomes and Biomedical Informatics
- 2021 o University of Hong Kong, Department of Computer Science
  - o University of Miami, College of Engineering
  - o Bristol Myers Squibb, Data Science
  - University of Washington, Genome Sciences Seminar
  - o ACM-BCB, Machine-learning Methods for Single-cell Analysis Workshop
  - International Conference on Machine Learning (ICML)
  - o International Conference on Intelligent Systems for Molecular Biology (ISMB)
- 2019 Cascadia Proteomics Symposium
  - ASMS Conference on Mass Spectrometry and Allied Topics
- 2016 Joint Statistical Meetings (JSM)

# **TEACHING**

# CS482/682 Computational Techniques in Biological Sequence Analysis, University of Waterloo.

- o Winter 2023, 2024
- o Enrollment: 60 students
- CS341 Algorithms, University of Waterloo.
  - Winter 2024
  - o Enrollment: 180 students

## STUDENT MENTORING

- 2023 present **Han Zhou**, *PhD student*.
  - o Cheriton School of Computer Science, University of Waterloo, Ontario, Canada
  - o Project: Disambiguated manifold alignment of single-cell data.
  - 2023 2024 **Fatemeh Alipour**, *PhD student*.
    - o Cheriton School of Computer Science, University of Waterloo, Ontario, Canada
    - Co-supervised with Prof. Lila Kari
  - 2023 2024 **Zhenbo Li**, *MMath student*.
    - o Cheriton School of Computer Science, University of Waterloo, Ontario, Canada
    - o Co-supervised with Prof. Bin Ma
  - 2019 2022 Winston Chen, Undergraduate student.
    - o School of Computer Science and Engineering, University of Washington, Seattle, WA, USA
    - o Project: Error-controlled interaction detection in deep neural networks.
    - Fall 2020 Timothy Yu, Rotational graduate student.
      - o Molecular and Cellular Biology Program, University of Washington, Seattle, WA, USA
      - o Project: Explaining single-cell cluster from an adversarial perspective.
    - Fall 2020 Chris Hsu, Rotational graduate student.
      - o Department of Genome Sciences, University of Washington, Seattle, WA, USA
      - Project: Designing sequence edits to change RNA splicing.
  - 2018 2020 **Jiaxing Bai**, *Master student*.
    - o Department of Automation, Xiamen University, Xiamen, China
    - Project: Learn the compact representations of metagenomic sequences.
  - 2018 2020 **Yiwen Wang**, *Master student*.
    - o Department of Automation, Xiamen University, Xiamen, China
    - Project: Automatic taxonomy embedding and categorization by Siamese triplet network.
  - 2016 2017 Kun Wang, Master student.
    - o Department of Automation, Xiamen University, Xiamen, China
    - o Project: Improving metagenomic binning by using alignment-free similarity measures.

# THESIS COMMITTEES

- 2025 **Zheng Ma**, PhD student.
  - o Cheriton School of Computer Science, University of Waterloo, Ontario, Canada
  - Thesis: "Advancing Proteomic Analyses with Graph-based Learning: Protein Inference and DIA De Novo Peptide Sequencing".
- 2025 **Shun Saito**, *PhD student*.
  - Cheriton School of Computer Science, University of Waterloo, Ontario, Canada
  - Thesis: "Modelling protein allostery using diffusion models".
- 2025 Monireh Safari, PhD student.
  - o Cheriton School of Computer Science, University of Waterloo, Ontario, Canada
  - Thesis: "LLM Foundational Models for Biodiversity Informatics and Environmental Signal Detection in Genomes".
- 2024 Jingjing Wang, Master student.
  - o Cheriton School of Computer Science, University of Waterloo, Ontario, Canada
  - o Thesis: "Multivariate Triangular Quantile Maps for Novelty Detection".

- 2024 **Shaokai Wang**, PhD student.
  - o Cheriton School of Computer Science, University of Waterloo, Ontario, Canada
  - Thesis: "Deep Learning Methods for Novel Peptide Discovering and Function Prediction".
- 2023 Pablo Millan Arias, PhD student.
  - o Cheriton School of Computer Science, University of Waterloo, Ontario, Canada
  - Thesis: "Deep Learning for Unsupervised Clustering of DNA Sequences".
- 2023 **Johra Moosa**, *PhD student*.
  - o Cheriton School of Computer Science, University of Waterloo, Ontario, Canada
  - Thesis: "Improving Peptide Identification in Proteomics Data Analysis through Repeat-Preserving Decoy and Decoy-Free Retraining".
- 2023 Shuyang Zhang, Master student.
  - o Cheriton School of Computer Science, University of Waterloo, Ontario, Canada
  - Thesis: "Spectrum and Retention Time Prediction for N-Glycopeptides Using Deep Learning".

# AWARDS AND SCHOLARSHIPS

- 08/2021 Most Innovative Presentation Award.
  - Machine-learning Methods for Single-cell Analysis Workshop, ACM-BCB 2021
- 2013–2015 **Provost's Fellowship**.
  - University of Southern California, Los Angeles, CA
- 2010–2013 **Graduate Fellowship**.
  - Shanghai Jiao Tong University, Shanghai, China
  - 2008 National Endeavor Scholarship.
    - Shanghai Jiao Tong University, Shanghai, China

# **SERVICES**

# SERVICE TO Associate Editor.

- PROFESSION PLOS Computational Biology, 2023–present
  - ACM Transactions on Probabilistic Machine Learning, 2023–present

#### Review Editor.

o Frontiers in Bioinformatics, Specialty Section of Single Cell Bioinformatics, 2022

## Area Chair.

- o IEEE/ACM International Conference on Connected Health: Applications, Systems, and Engineering Technologies (CHASE), 2025
- ACM Conference on Bioinformatics, Computational Biology and Biomedicine (ACM-BCB), 2024
- ACM Conference on Bioinformatics, Computational Biology and Biomedicine (ACM-BCB), 2023
- Al4Science Workshop, International Conference on Machine Learning (ICML), 2023

#### Program Committee.

- o Machine Learning in Computational Biology (MLCB), 2021
- Machine-learning Methods for Single-cell Analysis Workshop, ACM-BCB, 2021
- ISMB/ECCB Conference for the Computational Mass Spectrometry (CompMS), 2021, 2022

#### Journal Reviewer.

 Annals of Applied Statistics, Bioinformatics, BMC Bioinformatics, Briefings in Bioinformatics, Frontiers in Genetics, Genome Biology, IEEE/ACM Transactions on Computational Biology and Bioinformatics, IEEE Transactions on Neural Networks and Learning Systems, Journal of Proteome Research, Nature Biotechnology, Nature Communications, Nature Machine Intelligence, Nature Methods, Nucleic Acids Research, PLOS Computational Biology

# Conference Reviewer.

o AAAI, AISTATS, APBC, ICLR, ICML, ISMB, NeurIPS, RECOMB

# SERVICE TO **Graduate Committee**.

UNIVERSITY • Member, 2023–2024

# Nominating Committee for Director of School.

o Member, 2023–2024

# Graduate Recruiting Committee.

o Member, 2022–2023