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.

- o Computational genomics/proteomics/microbiomics
- Multi-omics integration
- o Bioinformatics analysis using large-language models

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

01/2023- University of Waterloo, Ontario, Canada.

Present o Assistant Professor at Cheriton School of Computer Science

01/2018- University of Washington, Seattle, WA, USA.

11/2022 \circ 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

PUBLICATIONS

 \ast indicates equal contribution. \dagger indicates the corresponding author.

PUBLICATIONS AS LEADING OR CORRESPONDING AUTHOR

- 1. W Chen, Y Jiang, WS Noble, and $\underline{YY Lu}^{\dagger}$. "Error-controlled non-additive interaction discovery in machine learning models". Under review, 2024.
- 2. Y Jiang, D Liao, Q Zhu, and YY Lu[†]. "PhyloMix: Enhancing microbiome-trait association prediction through phylogeny-mixing augmentation". bioRxiv:10.1101/2024.08.26.609661, 2024.
- 3. YY Lu, WS Noble, and U Keich. "A BLAST from the past: revisiting BLAST's E-value". bioRxiv:10.1101/2024.07.16.603405, 2024.
- 4. Z Dong, V Zhong, and $\underline{YY} \underline{Lu}^{\dagger}$. "BioMANIA: Simplifying bioinformatics data analysis through conversation". bioRxiv:10.1101/2023.10.29.564479, 2023.
- 5. Y Jiang, M Aton, Q Zhu † , and <u>YY Lu † </u>. "MIOSTONE: Modeling microbiome-trait associations with taxonomy-adaptive neural networks". bioRxiv:10.1101/2023.11.04.565596, 2023.
- 6. H Zhou, K Cao, and $\underline{YYLu}^{\dagger}$. "SONATA: Disambiguated manifold alignment of single-cell data". bioRxiv:10.1101/2023.10.05.561049, 2023.
- 7. W Chen, WS Noble[†], and YY Lu[†]. "DeepROCK: Error-controlled interaction detection in deep neural networks". arXiv:2309.15319, 2023.
- 8. Z Ma*, <u>YY Lu</u>*†, 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. YY Lu 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. YY Lu*, 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.
- 19. 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. 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". bioRxiv:10.1101/2023.02.22.529597, 2023.
- 2. 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.
- 3. 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.
- 4. 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.
- 5. 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.
- 7. 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.
- 8. 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.
- 9. 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.
- 10. 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.
- 11. NA Ahlgren, J Ren, 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.

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

o Role: PI

o Amount: \$167,500

INVITED LECTURES

- 2023 O Amgen, Data Sciences
 - Western University, Bioinformatics Seminar
 - University of Ottawa, Technologies for Microbiome Science and Engineering seminar
- 2022 HSE University, School of Data Analysis and Artificial Intelligence
 - University of Texas MD Anderson Cancer Center, Data Science and Modeling Forum
 - 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
 - Drexel University, College of Computing and Informatics
 - o National University of Singapore, Department of Biological Sciences
 - o Indiana University School of Medicine, Herman B Wells Center for Pediatric Research
 - o University of Florida, Department of Health Outcomes and Biomedical Informatics

- 2021 O University of Hong Kong, Department of Computer Science
 - University of Miami, College of Engineering
 - Bristol Myers Squibb, Data Science
 - University of Washington, Genome Sciences Seminar
 - o ACM-BCB, Machine-learning Methods for Single-cell Analysis Workshop
 - o 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.

- O Winter 2024
- Enrollment: 180 students

STUDENT MENTORING

2023 – present **Yifan Jiang**, *PhD student*.

- o Cheriton School of Computer Science, University of Waterloo, Ontario
- Project: Modeling microbiome-trait associations with taxonomy-adaptive neural networks.

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 – present **Zhengyuan Dong**, *PhD student*.

- o Cheriton School of Computer Science, University of Waterloo, Ontario, Canada
- Project: Simplifying bioinformatics data analysis through conversation.

2023 – present **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*.

- 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
- o 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
 - Project: Improving metagenomic binning by using alignment-free similarity measures.

THESIS COMMITTEES

- 2024 **Jingjing Wang**, *Master student*.
 - o Cheriton School of Computer Science, University of Waterloo, Ontario, Canada
 - Thesis: "Multivariate Triangular Quantile Maps for Novelty Detection".
- 2024 **Shaokai Wang**, PhD student.
 - o Cheriton School of Computer Science, University of Waterloo, Ontario, Canada
 - o 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.
 - Cheriton School of Computer Science, University of Waterloo, Ontario, Canada
 - o 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**.
 - o University of Southern California, Los Angeles, CA
- 2010–2013 **Graduate Fellowship**.
 - o 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.

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

Area Chair.

- o 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

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

REFERENCES

Prof. William S. Noble (Postdoc advisor)
Professor
Department of Genome Sciences and
School of Computer Science and Engineering
University of Washington
send.Noble.D3EF3353F6@interfoliodossier.com

Prof. **Uri Keich**Associate Professor
School of Mathematics and Statistics
University of Sydney
send.Keich.E4268BFC98@interfoliodossier.com

Prof. Ming Li University Professor Emeritus School of Computer Science University of Waterloo mli@uwaterloo.ca Prof. **Fengzhu Sun** (PhD advisor) Professor Department of Quantitative and Computational Biology and

Mathematics
University of Southern California
send.Sun.41F38EBF06@interfoliodossier.com

Prof. Michael S. Waterman
University Professor Emeritus
Department of Quantitative and Computational Biology, Mathematics, and Computer Science
University of Southern California
send.Waterman.A13F563250@interfoliodossier.com