Ziheng Duan

Department of Computer Science
Donald Bren School of Information and Computer Sciences
University of California, Irvine

duanziheng1206@gmail.com
+1 424 239 4085
zihengduan.cn

EDUCATION

Ph.D.   Computer Science, University of California, Irvine, 2021 - 2025 (expected)

M.S.   Computer Science, University of California, Irvine, 2021 - 2024

B.S.   Automation & Computer Science (Dual Degree), Zhejiang University, 2016 - 2020

RESEARCH INTERESTS

AI Methodologies: Graph Learning, Multimodal Modeling, Large Language Models
Biological Research: Single-Cell Genomics, Spatial Transcriptomics, Drug Discovery

WORK EXPERIENCE

Machine Learning Research Intern   Jun. 2025 – Present
Genesis Therapeutics, San Diego, CA
Developed KNOT: A Knowledge Graph and Omics Integration Framework for Target Identification, integrating multi-omics data and biomedical knowledge graphs to enhance drug target prediction.

Graduate Researcher   Sep. 2021 – Present
University of California, Irvine, CA
Developed trustworthy computational methods to understand single-cell gene regulation, especially in spatial contexts, and their contributions to various diseases.

PUBLICATIONS

First Author Publications

[9]   **Duan, Z.**, Li, X., Zhang, Z., Song, J., & Zhang, J. (2025). DISCO: A Diffusion Model for Spatial Transcriptomics Data Completion. *ICIP-2025: 2025 IEEE International Conference on Image Processing*.

[8]   **Duan, Z.**, Xu, S., Lee, C.Y., Riffle, D., & Zhang, J. (2024). iMIRACLE: an Iterative Multi-View Graph Neural Network to Model Intercellular Gene Regulation from Spatial Transcriptomic Data. *CIKM-2024: The 33rd ACM International Conference on Information and Knowledge Management*. doi:10.1145/3627673.3679574

[7]   **Duan, Z.**, Riffle, D., Li, R., Liu, J., Min, M. R., & Zhang, J. (2024). Impeller: a path-based heterogeneous graph learning method for spatial transcriptomic data imputation. *Bioinformatics*, btae339. doi:10.1093/bioinformatics/btae339

[6]   **Duan, Z.**, Xu, S., Sai Srinivasan, S., Hwang, A., Lee, C. Y., Yue, F., ... & Zhang, J. (2024). scENCORE: leveraging single-cell epigenetic data to predict chromatin conformation using graph embedding. *Briefings in Bioinformatics*, 25(2), bbae096. doi:10.1093/bib/bbae096

[5] **Duan, Z.**, Lee, C., & Zhang, J. (2023). ExAD-GNN: explainable graph neural network for Alzheimer's disease state prediction from single-cell data. *APSIPA Transactions on Signal and Information Processing*, 12(5). doi:10.1561/116.00000239

[4] **Duan, Z.**, Dai, Y., Hwang, A., Lee, C., Xie, K., Xiao, C., ... & Zhang, J. (2023). iHerd: an integrative hierarchical graph representation learning framework to quantify network changes and prioritize risk genes in disease. *PLoS Computational Biology*, 19(9), e1011444. doi:10.1371/journal.pcbi.1011444

[3] **Duan, Z.**, Xu, H., Wang, Y., Huang, Y., Ren, A., Xu, Z., ... & Wang, W. (2022). Multivariate time-series classification with hierarchical variational graph pooling. *Neural Networks*, 154, 481-490. doi:10.1016/j.neunet.2022.07.032

[2] **Duan, Z.**, Xu, H., Huang, Y., Feng, J., & Wang, Y. (2022). Multivariate time series forecasting with transfer entropy graph. *Tsinghua Science and Technology*, 28(1), 141-149. doi:10.26599/TST.2021.9010081

[1] **Duan, Z.**, Wang, Y., Ye, W., Fan, Q., & Li, X. (2022). Connecting latent relationships over heterogeneous attributed network for recommendation. *Applied Intelligence*, 52(14), 16214-16232. doi:10.1007/s10489-022-03340-7

Other Publications

[20] Hwang, A., Skarica, M., ..., **Duan, Z.**, ..., Zhang, J., & Girgenti, M. J. (2025). Single-cell transcriptomic and chromatin dynamics of the human brain in PTSD. *Nature*. doi:10.1038/s41586-025-09083-y

[19] Liu, J., Xu, S., Riffle, D., **Duan, Z.**, Min, M. R., & Zhang, J. (2024). Understanding Transcriptional Regulatory Redundancy by Learnable Global Subset Perturbations. *ACML-2024: Proceedings of the 16th Asian Conference on Machine Learning*, PMLR 260:383–398. openreview.net/forum?id=2ODI0B7Ijg

[18] Li, X., **Duan, Z.**, Dai, Y., Xu, S., & Zhang, J. (2024). iHAST: Integrating hybrid attention for super-resolution in spatial transcriptomics. In *Proceedings of the 35th British Machine Vision Conference (BMVC 2024)*. [PDF]

[17] Dai, Y., **Duan, Z.**, Xu, S., & Zhang, J. (2024). CytoFlow: a novel computational method to construct signal transduction networks at single-cell resolution based on flow networks. *MedAI-2024: IEEE International Conference on Medical Artificial Intelligence*, 212–217. doi:10.1109/MedAI62885.2024.00034

[16] Wen, C., Margolis, M., Dai, R., Zhang, P., Przytycki, P. F., Vo, D. D., ..., **PsychENCODE Consortium**, ... & Gandal, M. J. (2024). Cross-ancestry atlas of gene, isoform, and splicing regulation in the developing human brain. *Science*, 384(6698), eadh0829. doi:10.1126/science.adh0829

[15] Deng, C., Whalen, S., Steyert, M., Ziffra, R., Przytycki, P. F., Inoue, F., ..., **PsychENCODE Consortium**, ... & Pollard, K. S. (2024). Massively parallel characterization of regulatory elements in the developing human cortex. *Science*, 384(6698), eadh0559. doi:10.1126/science.adh0559

[14] Huuki-Myers, L. A., Spangler, A., Eagles, N. J., Montgomery, K. D., Kwon, S. H., Guo, B., ..., **PsychENCODE Consortium**, ... & Maynard, K. R. (2024). A data-driven single-cell and spatial transcriptomic map of the human prefrontal cortex. *Science*, 384(6698), eadh1938. doi:10.1126/science.adh1938

[13] Ruzicka, W. B., Mohammadi, S., Fullard, J. F., Davila-Velderrain, J., Subburaju, S., Tso, D. R., ..., **PsychENCODE Consortium**, ... & Kellis, M. (2024). Single-cell multi-cohort dissection of the schizophrenia transcriptome. *Science*, 384(6698), eadg5136. doi:10.1126/science.adg5136

[12] Emani, P. S., Liu, J. J., Clarke, D., Jensen, M., Warrell, J., Gupta, C., ..., **Duan, Z.**, ... & Gerstein, M. (2024). Single-cell genomics and regulatory networks for 388 human brains. *Science*, 384(6698), eadi5199. doi:10.1126/science.adi5199

[11] Dai, R., Chu, T., Zhang, M., Wang, X., Jourdon, A., Wu, F., ..., **PsychENCODE Consortium**, ... & Liu, C. (2024). Evaluating performance and applications of sample-wise cell deconvolution methods on human brain transcriptomic data. *Science Advances*, 10(21), eadh2588. doi:10.1126/sciadv.adh2588

[10] Pratt, H. E., Andrews, G., Shedd, N., Phalke, N., Li, T., Pampari, A., ..., **PsychENCODE Consortium**, ... & Weng, Z. (2024). Using a comprehensive atlas and predictive models to reveal the complexity and evolution of brain-active regulatory elements. *Science Advances*, 10(21), eadj4452. doi:10.1126/sciadv.adj4452

[9] Xia, Y., Xia, C., Jiang, Y., Chen, Y., Zhou, J., Dai, R., ..., **PsychENCODE Consortium**, ... & Chen, C. (2024). Transcriptomic sex differences in postmortem brain samples from patients with psychiatric disorders. *Science Translational Medicine*, 16(749), eadh9974. doi:10.1126/scitranslmed.adh9974

[8] Lee, C. Y., Riffle, D., Xiong, Y., Momtaz, N., Lei, Y., Pariser, J. M., ..., **Duan, Z.**, ... & Zhang, J. (2024). Characterizing dysregulations via cell-cell communications in Alzheimer's brains using single-cell transcriptomes. *BMC neuroscience*, 25(1), 24. doi:10.1186/s12868-024-00867-y

[7] Zhang, R., **Duan, Z.**, Lee, C. Y., Riffle, D., Min, M. R., & Zhang, J. (2023). Turtling: A Time-aware Neural Topic Model on NIH Grant Data. *Bioinformatics Advances*, vbad096. doi:10.1093/bioadv/vbad096

[6] Lee, C. Y., Chen, Y., **Duan, Z.**, Xu, M., Girgenti, M. J., Xu, K., ... & Zhang, J. (2022). Venus: An efficient v irus infection de tectio n and fu sion s ite discovery method using single-cell and bulk RNA-seq data. *PLOS Computational Biology*, 18(10), e1010636. doi:10.1371/journal.pcbi.1010636

[5] Wang, Y., **Duan, Z.**, Huang, Y., Xu, H., Feng, J., & Ren, A. (2022). MTHetGNN: A heterogeneous graph embedding framework for multivariate time series forecasting. *Pattern Recognition Letters*, 153, 151-158. doi:10.1016/j.patrec.2021.12.008

[4] Xu, H., **Duan, Z.**, Wang, Y., Feng, J., Chen, R., Zhang, Q., & Xu, Z. (2021). Graph partitioning and graph neural network based hierarchical graph matching for graph similarity computation. *Neurocomputing*, 439, 348-362. doi:10.1016/j.neucom.2021.01.068

[3] Liao, Z., Yang, Y., Sun, C., Wu, R., **Duan, Z.**, Wang, Y., ... & Xu, J. (2021). Image-based prediction of granular flow behaviors in a wedge-shaped hopper by combing DEM and deep learning methods. *Powder Technology*, 383, 159-166. doi:/10.1016/j.powtec.2021.01.041

[2] Wang, B., Zhou, C., **Duan, Z.**, Zhu, Q., Wu, J., & Xiong, R. (2020). Untethered quadrupedal hopping and bounding on a trampoline. *Frontiers of Mechanical Engineering*, 15, 181-192. doi:/10.1007/s11465-019-0559-5

[1] Wang, Y., **Duan, Z.**, Liao, B., Wu, F., & Zhuang, Y. (2019, July). Heterogeneous attributed network embedding with graph convolutional networks. *In Proceedings of the AAAI conference on artificial intelligence* (Vol. 33, No. 01, pp. 10061-10062). doi:10.1609/aaai.v33i01.330110061

INVITED TALKS

- "scENCORE, a computationally method to reconstruct chromatin compartments from the more affordable and widely accessible single-cell epigenetic data."
  13th Annual Symposium, Southern California Systems Biology   May 2024
- "iHerd, a hierarchical graph representation learning method for identifying key driver genes by analyzing gene network changes across different conditions."
  2023 SCORCH Consortium Meeting   Dec 2023

AWARDS AND HONORS

- Travel Grant, IEEE International Conference on Image Processing (ICIP 2025)   2025
- Dean's Fellowship, University of California, Irvine   2021
- Research and Innovation Scholarship, Zhejiang University   2019
- Academic Excellence Scholarship, Zhejiang University   2017 – 2019

TEACHING

- *Reader*, University of California, Irvine   Spring 2022
  ICS 6D: Discrete Mathematics for Computer Science
- *Reader*, University of California, Irvine   Winter 2021
  ICS 178: Machine Learning and Data Mining
- *Reader*, University of California, Irvine   Fall 2021
  ICS 178: Machine Learning and Data Mining

MENTORING

- *Mentor*, Google Summer of Code 2025   Summer 2025
  RAG-ST: Retrieval-Augmented Generation for Spatial Transcriptomics
  Guided the development of a retrieval-augmented framework for predicting spatial gene expression from histology images, focusing on interpretability and modular design.

- *Mentor*, Google Summer of Code 2024   Summer 2024
  BenchmarkST: Spatial Transcriptomics Gene Imputation Benchmarking
  Supervised the creation of a benchmarking suite for evaluating cross-platform, multi-species gene expression imputation methods.

SERVICES

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Learning on Graphs Conference (LoG)

The International Conference on Intelligent Systems for Molecular Biology (ISMB)

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