Zhiyu Wang

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AI4Biology | LLMs | AI Agents | Geometric Deep Learning

Education

University of Cambridge — Cambridge, UK
Advanced Computer Science, Master of Philosophy (Distinction, Rank: 8/60) — Oct 2024 — Jul 2025
- Courses: Geometric Deep Learning, Affective AI, Mobile & Wearable ML, NLP, Multi-agent RL

University College London — London, UK
Computer Science, Bachelor of Science (First Class Honors) — Sep 2021 — Jun 2024
- Main Courses: Machine Learning, Computer Vision, Reinforcement Learning, Mathematics & Statistics, Software Engineering

Publications

1. **"Fast and Interpretable Protein Substructure Alignment via Optimal Transport."**
   Zhiyu Wang*, Bingxin Zhou*, Jing Wang, Yang Tan, Weishu Zhao, Pietro Liò, Liang Hong. *ICLR*, 2026. (**arXiv:2510.11752**)
2. **"Topotein: Topological Deep Learning for Protein Representation Learning."**
   Zhiyu Wang, Arian Jamasb, Mustafa Hajij, Alex Morehead, Luke Braithwaite, Pietro Liò. *arXiv preprint*, 2025. (**arXiv:2509.03885**)
3. **"MoRE-GNN: Multi-omics Data Integration with a Heterogeneous Graph Autoencoder."**
   Zhiyu Wang, Sonia Koszut, Pietro Liò, Francesco Ceccarelli. *arXiv preprint*, 2025. (**arXiv:2510.06880**)
4. **"GraphAU-Pain: Graph-based Action Unit Representation for Pain Intensity Estimation."**
   Zhiyu Wang, Yang Liu, Hatice Gunes. *IJCAI 2025 MiGA Workshop*. (**arXiv:2505.19802**)

Research Experience

Protein Substructure Alignment via Optimal Transport | University of Cambridge & SJTU — Cambridge, UK
External collaboration | *Supervisor: Prof. Pietro Liò & Prof. Liang Hong* — Apr 2025 — Sep 2025
- Accepted at ICLR 2026 as a poster. (**Paper**)
- Developed PLASMA, a module based on optimal transport that can be seamlessly added to any protein representation learning model with minimal training or even no training to enable fast and highly accurate identification of locally similar substructures.
- Completed extensive experiments on 7 backbone protein language models across 3 tasks from the VenusX dataset (motifs, active sites, and binding sites), demonstrated consistant and significant improvement (+10-30% ROC-AUC) across all backbones and tasks.
- Conducted case studies using PyMol visualizations and proved that the founded similar substructures are indeed similar in structure and they are not found just because of sequence similarity.

Hierarchical Protein Representation Learning | University of Cambridge — Cambridge, UK
Masters thesis | *Supervisor: Prof. Pietro Liò* — Oct 2024 — Sep 2025
- Developed TCPNet, an SE(3)-equivariant topological neural network that simultaneously learns protein residue-level and secondary structure-level features without losing any geometric information. (**Invited Talk**) (**Paper**)
- Awarded Highly Commended M.Phil Project Prize 2024-2025 by the Department of Computer Science and Technology
- Demonstrated 5% improvement on average across 3 popular protein representation learning tasks when only structure features are provided, which can be particularly important for de novo antibody design.

Multi-Omics Integration Data with GNNs | University of Cambridge — Cambridge, UK
Course project | *Supervisor: Prof. Pietro Liò* — Feb 2025 — Sep 2025

- Using heterogeneous graph network for embedding single cell multi-omics (e.g. RNA, protein, and ATAC modalities) data to a shared latent space and conduct cell clustering. (**Paper**)
- Training time on BM-CITE and LUNG-CITE datasets takes less than an hour on a laptop GPU, with 3% lower ARI and 2% lower NMI compared to the statistical method MOJITOO.

Graph-based Pain Estimation from Facial Expresissions | University of Cambridge — Cambridge, UK
Course project | *Supervisor: Prof. Hatice Gunes* — Oct 2024 — Jan 2025

- Presented at IJCAI25 MiGA Workshop. (**Paper**)
- Proposed the GraphAU-Pain model that fuses a ResNet-50 backbone with graph-based facial action unit (AU) representation learning for pain intensity estimation, allowing better clinical interpretability and generalization compared to purely image-driven methods.
- Developed a novel transfer learning strategy to address domain differences and missing annotations, improving GraphAU-Pain's AU occurrence prediction F1-score by 30% on the UNBC dataset.

Readmission Prediction with Remote Patient Monitoring Data | University College London — London, UK
Final year project | *Supervisor: Prof. Ivana Drobnjak* — May 2023 — Jun 2024

- Collaborated with clinicians from UCL Hospital to develop a SQL-based data pipeline for processing raw remote patient monitoring data, performing clinical feature engineering, and building interpretable ML models (ROC-AUC 0.79±0.03) with `SHAP` analysis.
- Designed a patient-independent stratified bootstrapping evaluation framework to address extreme data scarcity (55 patients) and class imbalance, preventing data leakage and ensuring robust generalization estimates for clinical deployment.

Industrial Experience

AI Scientist & Timeseries Generation/Prediction | Sapient Intelligence — Beijing, China
ML Research Scientist — Sep 2025 — Present

- Developing Praxit, an autonomous AI-scientist framework with DAG-based execution lineage for solution provenance; achieved ∼30% higher performance at 10% of the cost of Claude Code with Opus on Karpathy's AutoResearch prompt.
- Showcased Praxit at **AI4 2026** through live booth demos and conversations with prospective customers and collaborators.
- Generating synthetic time-series data and developing **HRM**-based forecasting models for weight management applications.

Healthcare LLM Knowledge Distillation | Xunfei Healthcare Technology — Hefei, China
Intern ML Researcher — Jul 2024 — Sep 2024

- Built a knowledge distillation pipeline using a teacher LLM to synthesize medical instruction examples from human-annotated samples, improving student model (**Xiaoyi**) instruction-following accuracy from 34% to 82% via supervised fine-tuning.

RAG-Based Financial Intelligence System | Luojin Data Information — Shanghai, China
Intern ML Engineer — May 2023 — Aug 2023

- Developed a RAG pipeline with `MongoDB` vector store and `LangChain` agents for automated financial report classification, achieving 92% query translation accuracy and 97% entity matching rate through semantic search.

Low-cost AI Chatbot Generation System for Hospitals | National Health Service — London, UK
Intern Software Engineer — Sep 2022 — May 2023

- Created an automated chatbot generation service for hospitals, reducing development time from weeks to 30 minutes.
- Delivered a live demonstration at Great Ormond Street Hospital to clinicians, and presented at UCL to IBM, Microsoft, and Intel, earning **media recognition** from an IBM Master Inventor.

Additional Experience

- **Reviewer Experience:** NeurIPS 2026; AI4Science Workshop at NeurIPS 2025 and ICML 2026
- **Teaching Experience:** Programming Tutor at UCL (2022–23)