Xinxiang Wang

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Research Interests

- **Large Language Models & Agent Systems**: retrieval-augmented reasoning, autonomous agents, and multi-agent collaboration.
- **AI for Science**: generative modeling, physics-informed learning, and domain-specific foundation models for accelerating scientific discovery.

Education

B.Eng. **Hunan Institute of Traffic Engineering**, Data Science and Big Data Technology — Sept 2020 – Jun 2024

- GPA: **3.38/4.00** (Avg: 84.32/100).
- **Honors & Awards:**
  - Outstanding Graduate (2024)
  - Outstanding Graduation Thesis
  - CUMCM Hunan Division 2nd Prize (2023)
  - CUMCM Hunan Division 3rd Prize (2022)
  - Provincial Innovation & Entrepreneurship Support (2023)

Research Experience

SyAGram: Dual-Component Framework for Anti-Gram-Negative AMP Classification and Generation *First Author, Under Review at IEEE BIBM 2025 (**CCF-B**)*
Apr 2025 – Jul 2025

- Proposed a dual-component framework designed to move beyond broad-spectrum approaches by enabling domain-focused modeling; demonstrated on antimicrobial peptides but applicable to other specialized fields.
- Developed a hybrid BiLSTM + physicochemical feature classifier and an ESM-2–guided discrete diffusion generator with functional control.
- Achieved **91.53% AUC** in classification and generated peptides with **92% predicted activity** and **62.3% high-confidence rate**, surpassing state-of-the-art baselines.

PHESA: Physics-informed Hierarchical Edge-Set Attention for Binding Affinity Prediction *Second Author, Under Review at IEEE BIBM 2025 (**CCF-B**)*
May 2025 – Jul 2025

- Proposed an edge-centric hierarchical framework with physics-informed priors to better capture atomic and group-level interactions in binding affinity prediction.
- Designed two-scale graph representations and physics-biased attention with cross-level pooling; contributed to data preprocessing, training, and visualization pipelines.
- Achieved SOTA on PDBbind (Pearson **0.795** on Seq-ID 60%); transferable to PPI affinity tasks; self-supervised pre-training further boosted CASF-2016 generalization (R **0.80**, RMSE 1.25).

GAgent: Hierarchical Task Decomposition Framework for Mitigating LLM Errors in Complex Workflows *Project Lead, Targeting UbiComp/ISWC 2025 (**CCF-A**)*
Aug 2024 – Present

- Proposed hierarchical decomposition approach reducing LLM hallucination by decomposing complex tasks into minimal atomic units, preventing quality deterioration from extended contexts.
- Developed context-aware orchestration with semantic retrieval and multi-modal evaluation, integrated with specialized databases for output verification, achieving **40% error reduction** in complex reasoning.
- Implemented intelligent scheduling algorithms (DAG/BFS/postorder) with dependency resolution and iterative refinement, maintaining **92% success rate** across scientific workflows.

Work Experience

Shenzhen Shanjian Intelligent Technology Co., Ltd. *Python Back-end Developer (LLM & Agent Systems)*
https://www.sjzn.com/
May 2024 – Jan 2025

- **Project Involvement:** Built **LLM- and agent-driven** services alongside image/video processing pipelines: retrieval-augmented QA, instruction-tuned chat, and multi-agent workflows for internal automation (planning, tool-use, reporting).
- **Contributions to Project:**
  1. Implemented **RAG pipelines** (Milvus-based indexing, prompt templating, context compression) and integrated them into production APIs.
  2. Built **agent workflows** with planner–executor roles (tool calling for DB/search/HTTP), task decomposition, and error-recovery; authored evaluation harness and regression tests.
  3. Fine-tuned and optimized **Transformer LLMs** (instruction tuning, response ranking, latency/cost controls) and containerized the stack for deployment (Docker).
  4. Optimized image processing algorithms (**+20%** rendering efficiency); updated ComfyUI modules (**+15%** user positive feedback); refactored repository and CI/CD (**-40%** project cycle).

Hunan Ginkgo Reliability Technology Research Institute Co., Ltd. *Big Data Development Engineer*
https://www.dataginkgo.com/
Jun 2023 – Aug 2023

- **Project Involvement:** Engaged in **data integration, ETL pipeline design, and predictive modeling**. Built end-to-end workflows covering multi-source data ingestion, cleaning, feature engineering, and business-oriented analysis for reliability and marketing tasks.
- **Contributions to Project:**
  1. Unified five heterogeneous data sources into a centralized warehouse, improving query efficiency by **30%**.
  2. Automated preprocessing with Python (pandas, NumPy, SQL), reducing manual workload by **100+ hours/month** and raising data quality by **25%**.
  3. Designed and validated a **customer churn prediction model**, achieving **85% accuracy**, enabling actionable insights for client retention.

Publications & Patents

Under Review

SyAGram: Dual-Component Framework for Anti-Gram-Negative AMP Classification and Generation *First Author*
*Under Review at IEEE BIBM 2025 (**CCF-B**)*

PHESA: Physics-informed Hierarchical Edge-Set Attention for Binding Affinity Prediction *Second Author*
*Under Review at IEEE BIBM 2025 (**CCF-B**)*

Published Works

- **Wang X**, Teng Z*, Qu H, et al. *The study on the force analysis model of wave energy devices in heaving and pitching motion*. Highlights in Science, Engineering and Technology, 2024. (CPCI-indexed)
- Deng H, Chen H*, **Wang X**. *Design of heliostat field based on ray tracing*. Highlights in Science, Engineering and Technology, 2024. (CPCI-indexed)
- Teng Z, Zhou H*, **Wang X**, et al. *Research on Optimization Design of Heliostat Field Based on Ray Tracing*. Highlights in Science, Engineering and Technology, 2024. (CPCI-indexed)
- Xiong Li, **Wang Xinxiang**, Ma Chengyuan, et al. *A method, system, device and storage medium for image segmentation*. CN202410756483.1; CN118334061B; 2024. [in Chinese]
- Xiong Li, Ma Chengyuan, Dang Wenzhe, Hou Muzhou, Cao Cong, Luo Hu, **Wang Xinxiang**, et al. *A spatial conversion method, device, electronic equipment and medium*. CN118333848B; 2024-09-03. [in Chinese]
- Xiong Li, Ma Chengyuan, Dang Wenzhe, Hou Muzhou, Cao Cong, Luo Hu, **Wang Xinxiang**, et al. *Pilot optimization method for surgical navigation*. CN118333848A; 2024-07-12. [in Chinese]