Zirou Qiu

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Education

Ph.D. in Computer Science, University of Virginia — Aug 2020 – **Present**
Thesis Focus: Mathematical Optimization and Inference of Large Systems — Advisor: Madhav Marathe

M.S. in Computer Science, Clemson University — Aug 2018 - May 2020

B.S. in Computer Science, Southeast Missouri State University — Aug 2013 - May 2018

Select Work Experience

Biocomplexity Institute and Initiative - Research Assistant — *Sep 2020 – **Present** (Virginia)*

- Working in a **cross-disciplinary** team with over 40 scientists from fields such as CS, social science, and economics. Developed communication, project management, and teamwork skills within a large group.
- Researching the foundations of large-scale systems (e.g., social, multi-agent, infrastructure, and transportation systems) via **machine learning**, **optimization** and **mathematical modeling**. Served as the **lead** researcher in five projects, with **publications** at top venues (e.g., PNAS 22 & 23, AAMAS 23, AAAI 22, 23 & 24, ICML 22 & 24). Made important contributions to NSF Expeditions Project in Computing.
- Proposed a collection of novel and scalable **algorithms** and **analytical techniques** for optimizing and learning real-world systems, delivering both **near-optimal** theoretical performance guarantees, with state-of-the-art empirical results on the model accuracy and efficiency.
- Developing **large-scale formal frameworks** for multi-agent system simulation and data analysis using **Python** and tools such as **Spark**, **Networkx**, **Gurobi**, and **PyTorch**. Via experimentation, derived policy guidelines for effective decision-making and contributed to the projects at Biocomplexity Institute on pandemic prevention.

Fujitsu Research of America - Research Intern — *Sep 2024 – **Present** (Remote)*

- Investigating optimization problems for resource allocation and **motion planning** in quantum systems, a critical approach to enhance the efficiency of quantum algorithms on real-world quantum computers.
- Applying **graph representation learning** methods (e.g., GNN, clustering) and **reinforcement learning** methods to qubit mapping and routing problems, with the aim of optimizing hardware execution on physical devices.

Argonne National Laboratory - Research Intern — *May 2019 - Aug 2019 (Illinois)*

- Investigated optimization problems in large networks and developed novel **metaheuristics** to solve the network matching problem. The proposed algorithms achieved over **2 times** performance improvement compared to state-of-the-art methods. Published as first author at **ACM-JEA**.

Select Projects

Optimal Resource Planning and Allocation in Large-scale Systems — *Lead Researcher*
Biocomplexity Institute and Initiative — (2023 - **Present**)

- **Research Methods**: Optimization, game theory, mathematical modeling and simulation, network analysis
- Proposed **the first mathematical framework** for modeling spatial resource allocation on large networks. The framework encompasses a wide range of real-world allocation scenarios, from **facility allocation** to matching users on social platforms under diverse objectives.
- Developed novel and efficient optimization methodologies that are *provably* optimal, using techniques in **linear, integer, quadratic, dynamic and semidefinite programming**, **metaheuristics**, and **approximation** algorithms. Conducted comprehensive experiments with the models on real-world data using Python and Gurobi.
- One paper accepted at AAMAS-23, one paper in submission to PNAS.

Efficient Inference of Large Networked Systems — *Lead Researcher*
Biocomplexity Institute and Initiative — (2023 - **Present**)

- **Research Methods**: Machine learning on graphs, time series modeling, probabilistic analysis and inference.
- Proposed **the first** collection of effective, and highly scalable **learning algorithms** for black-box system

inference from **time series** data, under various real-world scenarios, such as learning for multi-layer networks or learning in high-noise environments. Established close-to-optimal performance guarantees with extensive empirical evaluations on the efficiency and effectiveness of the methods.

- Papers accepted at ICML-24, AAAI-24 and ICML-22. Two papers in submission to ICLR-25 and TCS.

Other Key Projects *Lead Researcher/Engineer*

- **Modeling and Simulation of Complex System Dynamics**: Designed **novel mathematical models** for simulating stochastic processes on large systems. Performed extensive simulations on real-world datasets, uncover novel system properties and behavioral patterns. Derived policy guidelines for pandemic prevention. Papers accepted at PNAS-23 and PNAS-22.
- **Optimization and Stability of Networked Systems**: Conducted comprehensive analyses on agent interactions in large systems. Proposed effective methods for **optimizing system stability**, and **addressed open problems** on the system convergence. Performed simulations to validate findings. Papers at AAAI-23 and AAAI-22.
- **Large-scale Market Modeling**: Building **a scalable system** to model decision-making in commodity markets (demand & supply, strategies, and trading). Applying the system on dataset of over **one million consumers**.
- **World models in LLM**: Building a benchmark dataset and a processing pipeline to investigate the world models in LLMs, including GPT, Claude, and LLaMA. Uncovered the limitations in the formal reasoning ability of LLMs, and proposed novel prompting techniques to improve the model performance. Completing one paper.

Select Papers

*I often use *dynamical systems* as a model for real-world complex systems (e.g., social, multi-agent, transportation systems).

[1] *Welfare Optimization for Resource Allocation with Peer Effects* [pdf] **In submission to PNAS**
Zirou Qiu, Daniel Rosenkrantz, Matthew O. Jackson, Simon Levin, S. S. Ravi, Richard Stearns, Madhav Marathe

[2] *Learning Discrete Dynamical Systems under Classification Noise* [pdf] **In submission to ICLR-25**
Zirou Qiu, Zakaria Mehrab, Abhijin Adiga, Madhav Marathe, S.S. Ravi, Dan Rosenkrantz, Richard Stearns, and Anil Vullikanti

[3] *Theoretical Foundations for Parent Divorcing in Bayesian Networks* [pdf] **In submission to TCS**
With Daniel Rosenkrantz, Madhav Marathe, and S.S. Ravi

[4] *Efficient PAC Learnability of Dynamical Systems Over Multilayer Networks* [pdf] **ICML-24** (Acc: 27.8%)
Zirou Qiu, Abhijin Adiga, Madhav Marathe, S.S. Ravi, Daniel Rosenkrantz, Richard Stearns, and Anil Vullikanti

[5] *Learning the Topology and Behavior of Discrete Dynamical Systems* [pdf] **AAAI-24** (Acc: 23.8%)
Zirou Qiu, Abhijin Adiga, Madhav Marathe, S.S. Ravi, Daniel Rosenkrantz, Richard Stearns, and Anil Vullikanti

[6] *Assigning Agents to Increase Network-Based Neighborhood Diversity* [pdf] **AAMAS-23** (**Oral**, Acc: 23.3%)
Zirou Qiu, Andrew Yuan, Chen Chen, Madhav Marathe, S.S. Ravi, Daniel Rosenkrantz, Richard Stearns, Anil Vullikanti

[7] *Airborne disease transmission during indoor gatherings* [pdf] **PNAS-23** (Acc: 14.7%)
Avinash Dixit, $^{(\alpha\text{-}\beta)}$ Baltazar Espinoza, **Zirou Qiu**, Anil Vullikanti, and Madhav Marathe

[8] *Networked Anti-Coordination Games Meet Graphical Dynamical Systems* [pdf] **AAAI-23** (**Oral**, Acc: 19.6%)
Zirou Qiu, Chen Chen, Madhav Marathe, S.S. Ravi, Daniel Rosenkrantz, Richard Stearns, and Anil Vullikanti

[9] *Understanding the Co-evolution of Mask-wearing and Epidemics* [pdf] **PNAS-22** (Acc: 14.7%)
Zirou Qiu, Baltazar Espinoza, Vitor V. Vasconcelos, Chen Chen, Sara M. Constantino, Stefani A. Crabtree, Luojun Yang, Anil Vullikanti, Jiangzhuo Chen, Jörgen Weibull, Kaushik Basu, Avinash Dixit, Simon Levin, Madhav Marathe

[10] *Learning Networked Dynamical Systems Via Active Queries* [pdf] **ICML-22** (**Spotlight**, Acc: 22%)
Daniel Rosenkrantz,$^{(\alpha\text{-}\beta)}$ Abhijin Adiga, Madhav Marathe, **Zirou Qiu**, S.S. Ravi, Richard Stearns, and Anil Vullikanti

[11] *Finding Nontrivial Minimum Fixed Points in Dynamical Systems* [pdf] **AAAI-22** (**Oral**, Acc: 15%)
Zirou Qiu, Chen Chen, Madhav Marathe, S.S. Ravi, Daniel Rosenkrantz, Richard Stearns, and Anil Vullikanti

Skills

Engineering: C/C++, Python, MATLAB, R, Node.js, PyTorch, TensorFlow, Scikit-Learn, Hugging face, MXNet, PEFT, FSDP, Transformers, LoRA, Docker, Anaconda, Git, AWS, CUDA, Spark, Linux, Optuna, Gurobi, SQL.

Research: Optimization, operations research, machine learning, deep learning, large language model, generative AI, design & analysis of algorithms, discrete math, game theory, large-scale modeling and simulation