Zirou Qiu

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Research Interest

My research advances the foundation of **large-scale complex systems** represented as graphs (e.g., social networks, multi-agent systems, infrastructure and transportation systems) through the lens of machine learning, optimization, computational modeling, network science and game theory.

I develop **formal computational models and techniques** to simulate, analyze and optimize large real-world systems, aiming to improve system performance, unveil system behaviors, and benefit the social good. I have performed extensive research on topics such as fairness in social systems, complex system optimization, routing, and planning, optimal resource allocation, agent-based modeling, and black-box system inference.

Select Research Projects and Papers [All publications]

*Note: I often use *dynamical systems* as a mathematical model for complex systems. However, the problems, techniques, and results in my work extend to the much border realm of real-world systems (e.g., social, multi-agent, and infrastructure systems).

Project I: Optimal Resource Planning and Allocation in Large-scale Systems

Lead Researcher

- **Project goal**: Design formal computational models and methodologies for *optimal* resource planning and allocation in real-world large-scale systems represented as graphs.
- **Methods**: Optimization, game theory, mathematical modeling and simulation, network analysis
- Proposed various frameworks for modeling resource allocation in complex systems.
- Developed efficient allocation strategies that are *provably* optimal or near-optimal, while accounting for fairness and diversity constraints.
- Conducted comprehensive agent-based simulations for resource allocation in large systems.

Project Outcomes:

[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*

- Developed a principled model for resource allocation with externalities (e.g., mutual influences among the resources or the population) in complex systems.
- Proposed efficient strategies that guarantees optimal or near-optimal welfare outcomes for real-world resource allocation scenarios.

[2] Assigning Agents to Increase Network-Based Neighborhood Diversity [pdf] ***AAMAS-23*** *(Acc: 23.3%)*

Zirou Qiu**, Andrew Yuan, Chen Chen, Madhav Marathe, S.S. Ravi, Daniel Rosenkrantz, Richard Stearns, Anil Vullikanti* (Oral***)

- Developed a formal model for real-world spatial resources allocation problems, such as public housing assignment and urban spatial planning, and inventory placement.
- Presented rigorous methodologies for resource allocation with provable close-to-optimal guarantees, while ensuring social diversity and fairness.

Project II: Efficient Inference of Complex Systems

Lead Researcher

- **Project goal**: Develop efficient algorithms and techniques for analyzing and learning large-scale complex systems represented as graphs (e.g., social systems, dynamical systems and multi-agent systems).
- **Methods**: Machine learning on graphs, sequential modeling, probabilistic analysis and inference, empirical evaluation on heterogeneous datasets.
- Proposed several efficient, effective, and highly scalable learning methods for black-box system inference.
- Established performance guarantees of the proposed methods both theoretically and experimentally.

Project Outcomes:

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

- Proposed efficient noise-tolerant algorithms for learning the behaviors of large-scale systems in realistic noisy environments, with a provable high learning accuracy.
- Our algorithms are highly scalable to large networks, and the amount of training data required is provably near-optimal.

[2] Theoretical Foundations for Parent Divorcing Transformations [pdf] ***In submission to TCS***
With *Daniel Rosenkrantz, Madhav Marathe, and S.S. Ravi*

- Estabilished a theoretical groundwork for dimensionality reduction in Bayesian inference.
- Proposed efficient algorithms for dimensionality reduction with provable guarantees.

[3] 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*

- Proposed the first efficient learning method for inferring the behaviors of large-scale multilayer social systems and multi-agent systems.
- Our algorithm achieves a high learning accuracy both theoretically and empirically. Further, the amount of training data required is provably near-optimal.
- Develop the foundations of learning multilayer complex systems with an exact analysis of the model complexity and expressiveness.

[4] 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*

- Investigated the core principles of learning both the behaviors and the topology of black-box social systems and multi-agent systems.
- Proposed several efficient learning algorithms with provable guarantees for real-world scenarios of learning large complex systems.

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

- Developed the first collection of active learning based methods for inferring both the behaviors and the topology of black-box social systems and multi-agent systems.
- Conducted an extensive experimental study on the empirical performs on the proposed algorithms on real-world networks over various learning scenarios.

Project III: Modeling and Simulation of Complex Systems
Lead Researcher

- **Project goal**: Advance the understanding of real-world complex systems by modeling various intricate dynamic processes and uncovering novel properties of systems via (agent-based) simulation.
- **Methods**: Computational (sequential) modeling, large-scale simulation and data analysis
- Designed principled models for multi-contagion diffusion on complex systems.
- Performed extensive simulations for dynamic processes over large systems on real datasets.
- Revealed novel phenomena and intrinsic properties of complex system dynamics.
- Derived policy guidelines for betterment of social good.

Project Outcomes:

[1] Airborne disease transmission during indoor gatherings over multiple time scales [pdf] ***PNAS-23***
Avinash Dixit, Baltazar Espinoza, ***Zirou Qiu****, Anil Vullikanti, and Madhav Marathe*

- Introduced a principled modeling framework that couples the fast dynamics of viral loads in the local scale and the slow dynamics of disease progression at the population level.
- Derived policy guidelines to lessen the negative impact of epidemics.

[2] Understanding the Co-evolution of Mask-wearing and Epidemics [pdf] ***PNAS-22***

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*

- Presented a fundamental model for dueling dynamics of social and biological contagions both cooperating and completing in a population.
- Conducted extensive agent-based simulations. Through our modeling, we uncovered a collection of previously unknown properties of contagion dynamics.
- Derived corresponding policy guidelines to suppress epidemics and prevent their resurgence.

Project IV: Dynamics and Stability of Complex Systems

Lead Researcher

- **Project goal**: Build the foundations of stochastic behavior and stability of complex systems.
- **Methods**: Mathematical (sequential) modeling, optimization, game theory
- Conducted rigorous analytical studies of diffusion in complex systems.
- Performed extensive agent-based simulations of dynamic processes on complex systems.

Project Outcomes:

[1] Networked Anti-Coordination Games Meet Graphical Dynamical Systems [pdf] ***AAAI-23*** *(Acc: 19.6%)*

Zirou Qiu, *Chen Chen, Madhav Marathe, S.S. Ravi, Daniel Rosenkrantz, Richard Stearns, and Anil Vullikanti* (***Oral***)

- Presented a formal groundwork for stability and convergence in real-word strategic situations such as resources sharing and competition within a society.
- Addressed a collection of previously open problems, including a result showing the fast convergence of the dynamics and finding a Nash equilibrium in graphical games.

[2] Finding Nontrivial Minimum Fixed Points in Networked Dynamical Systems [pdf] ***AAAI-22*** *(Acc: 15%)*

Zirou Qiu, *Chen Chen, Madhav Marathe, S.S. Ravi, Daniel Rosenkrantz, Richard Stearns, and Anil Vullikanti* (***Oral***)

- Established the principles of finding equilibrium points in contagion diffusion within a population, with the goal of minimizing the overall scale of infection in a society.
- Presented several efficient and effective algorithms on finding such equilibrium points with minimum numbers of infections.

Other ongoing key projects

Lead Researcher / Engineer

- **Large-scale Market Modeling**
  - Building a scalable system to model large commodity markets, incorporating components such as demand & supply, consumers & producers, strategies, and trading mechanisms.
  - Applying the system on large-scale dataset of over 1 million consumers.
  - Working with the software team at biocompleixy institute on designing software, system architecture, and agent based methodology.
- **World models in LLM**
  - Building a benchmark dataset of games to investigate the emergent world models in LLM including GPT, Claude, LLaMA and Mistral. Finishing one paper .

Research Experience

Biocomplexity Institute and Initiative *Mentors: S. S. Ravi, Dan Rosenkrantz, Dick Stearns*

Research Assistant at the Network Systems and Advanced Computing Division *Sep 2020 – **Present** (Virginia, US)*

- Working with a team of over 40 scientists from various domains such as CS, social science, and economics.
- Researching the foundations of complex systems from the perspective of computational modeling, optimization, machine learning, and game theory.
- Developing large-scale frameworks for socio-technical system modeling and data analysis using Python and tools such as spark, networkx, CPLEX, Gruobi, ArcGIS.

- The lead researcher in four research projects, all resulted in multiple publications (see Select Projects and Papers Section).
- Eight published works (PNAS 22 & 23, AAMAS 23, AAAI 22, 23, & 24, ICML 22 & 24), plus three in-submission papers. Made important contribution to the prestigious NSF Expeditions Project in Computing.

Fujitsu Research of America *Supervisors: Ankit Kulshrestha, Xiaoyuan Liu*

Research Intern at the Quantum Group *Sep 2024 – **Present** (Remote, US)*

- Investigating the problem of optimal resource allocation and routing in infrastructure systems by building mathematical models and optimization.
- Applying graph representation learning methods (e.g., GNN, clustering) to the qubit mapping problem.

Clemson University *Advisor: Ilya Safro*

Graduate Research Assistant at the Algorithms and Computational Science Lab *Jan 2019 - May 2020 (South Carolina, US)*

- Investigated computational problems in network science and biology.
- Built a pipeline for microbiome modeling. Discovered novel microbiome migration pattern.
- Collaborated with biologists from Argonne National Lab and UChicago.

Argonne National Laboratory *Host: Chris Henry*

Graduate Research Aide at the Data Science Division *May 2019 - Aug 2019 (Illinois, US)*

- Performed comprehensive analysis of microbiome data.
- Investigated the network alignment problem with applications in computational biology.
- One first-author published work at ACM-JEA.

Education

University of Virginia *Charlottesville, USA*

Ph.D. Candidate in Computer Science (GPA: 4.0) - Advisor: Madhav Marathe *Aug 2020 – **Present***

Clemson University *Clemson, USA*

M.S. in Computer Science (GPA: 3.75) - Advisor: Ilya Safro *Aug 2018 - May 2020*

Southeast Missouri State University *Cape Girardeau, USA*

B.S. in Computer Science (GPA: 3.7) - Dean's List, Cum Laude *Aug 2013 - May 2018*

Skills

Research: Machine learning, optimization, large-scale system modeling, mathematical modeling and programming, computational methods, network science, social network analysis, algorithm design and analysis, game theory, deep learning, foundation models, generative AI

Languages: C/C++, Python, MATLAB, R, React.js, Node.js, PHP

Frameworks and Tools: PyTorch, TensorFlow, Scikit-Learn, Hugging face, DeepSpeed, Megatron-LM, MXNet, PEFT, FSDP, Transformers, LoRA, Docker, Anaconda, Git, AWS (SageMaker), Pandas, Numpy, CUDA, Spark, Linux Bash, Optuna, Gurobi, SQL, Mathematica, ArcGIS Pro, Laravel, Tailwind CSS, npm