



**Department of Data Science & Institute for Data Science**  
**Faculty Candidate Seminar Talk**

## **Decision Making for Scientific Discovery: From Causal Inference to Reinforcement Learning**

by  
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**Hosted by Mengjia Xu**

**DATE:** Monday, March 4, 2024

**TIME:** 10:30pm-11:30pm

**LOCATION:** GITC 4402 (4th floor lecture hall)

**Zoom:** <https://njit-edu.zoom.us/j/964498892688?pwd=RFJyOEJaWXZlTXFQNIUzWnBpT3gxQT09>

**Passcode:** 214768

**Abstract:**

Artificial Intelligence (AI) is launching a new era of transformative scientific discovery, offering opportunities for accelerated discoveries in fields as critical as drug design and pandemic prevention. Central to these advancements is the ability to make informed decisions—a domain where much potential remains untapped.

In this talk, I will present my doctoral research on the application of AI in scientific and healthcare domains. I will begin by detailing how causal inference helps understand the impact of public policy such as traffic control decisions on pandemic transmission dynamics in various geographic regions. This method provides insights into the causal relationships between policy interventions and outcomes, serving as a foundation for data-driven decision-making.

Transitioning to the necessity of discoveries for future scientific endeavors, I will introduce the application of reinforcement learning (RL) to exploration and learning in uncertain environments. Emphasizing unsupervised RL, I will discuss how this approach facilitates the collection of informative data without predefined rewards, illustrating its potential through applications in robotics and beyond.

The talk concludes by showcasing the use of RL in scientific discovery and healthcare, from analyzing chemical reactions to predicting molecular structures, and outlines several promising future research directions in the AI for science domain.

**Bio:**

Weitong Zhang is in his dissertation year as a Ph.D. candidate in Computer Science at UCLA, where he is advised by Professor Quanquan Gu. His research interests mainly lie in AI for scientific discovery, particularly focusing on the foundation and practical applications of Reinforcement Learning within this scope. He is a recipient of the Amazon Fellowship, the UCLA Summer Research Fellowship, and the Dissertation Year Fellowship. He has also completed two research internships at Nvidia, where he contributed to projects on molecule generation and prediction for drug design. Prior to his doctoral studies, Weitong earned his bachelor's degree from the Department of Automation at Tsinghua University.