



# THE UNIVERSITY OF CHICAGO

Department of Statistics

## STATISTICS COLLOQUIUM

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ERIC JONAS

Department of Computer Science  
University of Chicago

### Machine Learning for Molecular Inverse Problems

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Via Zoom

#### ABSTRACT

Inverse problems are a well-studied branch of applied mathematics where we attempt to invert a reasonably-accurate forward model in an attempt to learn the properties of some hidden source. While tremendous progress has been made on linear inverse problems, the situation is more challenging for inverse problems where we are attempting to recover a structured object, such as a graph. Here I will describe our recent work on this class of problem with regards to molecular spectroscopy. In spectroscopic measurements, we attempt to completely recover the edges of a graph based on various local properties, such as per-vertex parameters or aggregating functions over graph partitions. We discuss means of approximating the quantum-chemical forward models, techniques from structured prediction for inverting the resulting models, and ways in which we might modify spectroscopic measurements to make the recovery easier.

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For further information and inquiries about building access for persons with disabilities, please contact Jonathan Rodriguez at 773.702.8333 or send him an email at [jgrodriquez@galton.uchicago.edu](mailto:jgrodriquez@galton.uchicago.edu). If you wish to subscribe to our email list, please visit the following website:  
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