THE UNIVERSITY OF CHICAGO

COMPUTATIONAL AND APPLIED MATHEMATICS
STUDENT SEMINAR

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Machine Learning for Molecules: Mass Spectrometry as a Case Study

Tuesday, January 19, 2021, 3:00 PM (Chicago Time)
Zoom Meeting ID: 972 4989 6395
Password: 673056

ABSTRACT

Mass spectrometry is a powerful analytical tool, helping chemists and biologists identify unknown molecules, characterize purity, and much more. Massive databases of experimental mass spectra have been collected for the hundreds of thousands of molecules of current interest - but there are many millions more of potentially interesting molecules with unobserved spectra. In order to unlock this data, we need to build efficient inverse models to go from measured spectra to candidate compounds. In this talk, we cover recent advances in machine learning for molecules, as well as how it can potentially lead to in silico mass spectrometry and accelerate experimentation.