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Tackling Spectroscopic Inverse Problems via Structured Prediction

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Jones 303, 5747 S. Ellis Ave. Chicago, IL 60637
OR
via Zoom

Spectroscopic measurements of molecules and mixtures can be viewed as inverse problems, where we often have good knowledge of the forward (measurement) process, and wish to recover unknowns (such as mixture concentrations or molecular structure). However, the measurement process is highly nonlinear (quantum mechanical) and the answers we seek have considerable structure and constraints (such as points on a simplex or discrete connected graphs). Here we will discuss our recent efforts at accurately computing the forward model for one such spectroscopic technique, mass spectrometry (MS). MS fragments molecules and measures the resulting charge-to-mass ratio of the resulting fragments, and is famously difficult to simulate ab initio. Using a novel graph-subset machine learning technique we can reduce the error in spectrum calculation by a factor of 3x and approach experimental-level accuracy, enabling us to begin tackling the inverse problem Time permitting, I will discuss our plans to extend this technique to newer MS instrumentation and opportunities for multiplexed dataset generation. Joint work with CAM student Richard Zhu.