BAYESIAN DEEP LEARNING MODELS FOR COMPLEX MIXTURE ANALYSIS

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With the development of high resolution and high bandwidth microwave spectrometers, we have reached a state where unbiased spectral line surveys of completely unknown mixtures can be systematically deconvolved, given sufficient time and effort. In our recent work on various discharge mixtures of benzene, we have shown that spectra comprising up to 220 distinct spectral carriers—including vibrationally excited states and isotopic species, with $\sim$60 species unknown prior to this work—can be gradually disentangled following weeks of fervent analysis. As we progress to increasingly complex and unknown mixtures, rotational spectra will become proportionally complicated and congested; conventional spectroscopic analysis cannot match the pace of data collection in astronomical observations and laboratory experiments.

In this talk, I will detail some efforts in our group of the recent months that leverage high-speed computation afforded by deep learning models. Inspired by the work of Zaleski and Prozument (2018), we sought to develop probabilistic deep learning models that are able to spectrally deconvolve multi-component spectra in an automated fashion. Within a Bayesian framework, these models are designed to operate with minimal information, requiring only spectral frequencies, and estimates the likelihood of sequences of frequencies originating from the same carrier. In addition to a description of the models, I will discuss how these models act as companions for spectral analysis, converting the typical user workload from a process of trial and error to one of statistical inference.