Can Machine Learning help us to systematically analyze the UV Resonance Raman Spectra of Glycoproteins absorbing on Nanoparticles?

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Abstract

We apply Gaussian Process (GP) regression to UV Resonance Raman (UVRR) Spectra of two glycoproteins, Fetuin and Asialofetuin, which differ only for the sialic acid end of their glycans. First, we collect their UVRR Spectra for temperatures ranging from 295 K to 359 K, at different concentrations, in bulk or with Carbon nanoparticles. Next, we characterize the spectra features under different conditions. Our findings show that GPs can reach state of the art in predicting the (noisy) experimental spectra, using suitable kernel functions depending on a few hyperparameters. More importantly, the GPs yield results amenable to sound physical interpretations that might lead to a novel machine learning protocol for a systematic analysis of UVRR spectra of proteins in the presence of nanoparticles.