# Novel Statistical Tools for Single Molecule Biophysics: A foray into Bayesian nonparametrics

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One route to modeling biophysical dynamics involves the bottom-up, molecular simulation, approach. In this approach, approximate classical potentials are used to simulate short time local motions in order draw insight on dynamics at longer time and larger length scales. Here we take a different route. Instead we present a topbottom approach to building models of single molecule conformational dynamics and diffusion. The approach we present exploits a novel branch of Statistics – called Bayesian nonparametrics (BNPs) – first proposed in 1973 and now widely used in data science as the important conceptual advances of BNPs have become computational feasible in the last decade. BNPs are new to the physical sciences. They use flexible (nonparametric) model structures to efficiently learn models from complex data sets. Here we will show how BNPs can be adapted to address important questions in biophysics directly from the data which is often limited by factors such as finite photon budgets as well as other fluorophore artifacts in addition to data collection artifacts (e.g. aliasing, drift). More specifically, we will show that BNPs hold promise by allowing complex spectroscopic time traces (e.g. smFRET, photon arrivals) or images (e.g. single particle tracking) to be analyzed and turned into principled models of single molecule motion – from diffusion to conformational dynamics and beyond.