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# Bayesian inferencing and deterministic anisotropy for molecular geometry retrieval in gas phase diffraction experiments

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Ultrafast molecular gas phase diffraction is a vital tool for retrieving time dependent molecular structures. We are limited in the systems we can study as we generally require complex molecular dynamics simulations to interpret the results. We develop an alternative analysis to approximate the molecular geometry distribution $|\Psi(\mathbf{r},t)|^2$ that does not require such complex simulations. We achieve real-space resolutions of 1 pm to 10 fm while uniquely defining the molecular structure. We demonstrate our method's viability by retrieving the ground state geometry distribution $|\Psi(\mathbf{r})|^2$ for simulated stretched $NO_2$ and measured $N_2O$. Our method expands the capabilities of ultrafast molecular gas phase diffraction to measure other variables, like the width of $|\Psi(\mathbf{r},t)|^2$. By not relying on complex simulations and with the order 100 fm resolution, our method has the potential to effectively turn ultrafast molecular gas phase diffraction into a discovery oriented technique, exploring systems that are prohibitively difficult to simulate.

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