

## Bayesian Inverse Problems and Their Use in Molecular Dynamics

*Thursday 29 August 2024 15:30 (1 hour)*

First, we will briefly introduce the basics of statistical inversion, where, in its most basic form, the goal is to study how to estimate model parameters from data. We will introduce mathematical concepts and computational tools for systematically treating these inverse problems in a Bayesian framework, including assessing how uncertainties affect the solution. In the second part, we will discuss an exemplary application of the Bayesian framework, which is pertinent to molecular dynamics. Specifically, we consider Bayesian inference for diffusion processes based on data available as (a collection of) stochastic trajectories or statistics like expectation values or probability distributions.

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