Sampling from a probability distribution is a fundamental algorithmic problem. We discuss applications of sampling to several areas including machine learning, Bayesian statistics and optimization. In many situations, for instance when the dimension is large, such sampling problems become computationally difficult.

Markov chain Monte Carlo (MCMC) algorithms are among the most effective methods used to solve difficult sampling problems. However, most of the existing guarantees for MCMC algorithms only handle Markov chains that take very small steps and hence can oftentimes be very slow. Hamiltonian Monte Carlo (HMC) algorithms – which are inspired from Hamiltonian dynamics in physics – are capable of taking longer steps. Unfortunately, these long steps make HMC difficult to analyze. As a result, non-asymptotic bounds on the convergence rate of HMC have remained elusive.

In this talk, we obtain rapid mixing bounds for HMC in an important class of strongly log-concave target distributions encountered in statistical and Machine learning applications. Our bounds show that HMC is faster than its main competitor algorithms, including the Langevin and random walk Metropolis algorithms, for this class of distributions.

Finally, we consider future directions in sampling and optimization. Specifically, we discuss how one might design adaptive online sampling algorithms for applications to problems in reinforcement learning and Bayesian parameter inference in partial differential equations. We also discuss how Markov chain algorithms can be used to solve difficult non-convex sampling and optimization problems, and how one might be able to obtain theoretical guarantees for the MCMC algorithms that can solve these problems.