663 Final Project Outline

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1 Abstract

For our project we will use Neal's 2011 paper, "MCMC using Hamiltonian dynamics." The paper discusses how to use Hamiltonian dynamics as a sampling scheme to explore target spaces better than traditional Metropolis-Hastings algorithms. The Hamiltonian is the sum of potential energy (based on position) and kinetic energy (based on momentum) - Hamilton's equations relate the two partial derivatives of the Hamiltonian to each other, and define a mapping from the state at time t to the state at time $t + s$. In Hamiltonian Monte Carlo (HMC), we draw auxiliary momentum variables from a Gaussian distribution, and use Hamiltonian dynamics simulations to update the position variable (which follows the distribution of interest). At the end of a user-defined number of steps of simulation, the new variables are accepted or rejected in a Metropolis-Hastings step.

In this report we will explore basic HMC with the "Leapfrog" discretization method, and follow some examples (such as highly-correlated multivariate Gaussian distributions) comparing HMC to random-walk Metropolis Hastings that show improvement for HMC. We will also implement an extension of HMC proposed by Neal (1994) that uses "windows" of states to allow for a high probability of acceptance for all trajectories. Finally, we plan on converting the code to Cython to speed up implementation, and compare to existing HMC packages.