Notes for Hoffman and Gelman. "The No-U-Turn Sampler: Adaptively Setting Path Lengths in Hamiltonian Monte Carlo"

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1. Introduction

MCMC can be used to draw samples that will converge in its distribution to the target distribution. MCMC methods can be less efficient than classic methods, but are more general and unbiased.

Hailtonian MCMC transforms the problem of sampling from a target distribution to simulating Hamiltonian dynamics. This is more efficient than a random-walk Metropolis algorithm, but it requires the gradient of the log-posterior and it needs a step size and number of leapfrog steps. Setting these two parameters can be difficult and expensive, requiring tuning runs first to determine the number of steps. The No-U-Turn Sampler (NUTS) can determine theses two parameters for us, eliminating the need for tuning runs and hand tuning.

2. Hamiltonian Monte Carlo

HMC works by also having momentum variables for every model parameter, which are independently drawn from a normal distribution. It works like a Hamiltonian physical system with the position, momentum, potential energy, kinetic energy and negative energy for a particle. The leapfrog integrator is used to evolve the system over time and update parameter proposals.

The performance for a HMC is dependant upon the choice of step size and step number. For too large step sizes the the simulation will be inaccurate and the result will be a low acceptance probability and if it is too small computations are wasted by taking a lot of small steps. For too small step number the samples will be close to each other and we will have a random-walk behavior and if it is too large then the HMC will loop back on itself and either explore parameter space very slowly or get stuck.

NUTS can calculate when the particle simulation has gone for long enough so these problems do not occur. A binary tree of points is made forwards and backwards in fictions time until the leftmost and rightmost nodes start to turn back on themselves (U-turn), That is the distance between them start to decrease.