Markov Chain Monte Carlo using Hamiltonian Dynamics

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Performance of MCMC

- MCMC is used to simulate a dependent sample from intractable distributions
- Performance as dimension grows is important with the rise of Big Data
- How far can we move with each proposal while keeping a optimal acceptance rate

Motivation for HMC

Algorithm	Scaling	Optimal Acceptance Rate ($d \to \infty$)
RWM	$d^{-1/2}$	23.4% (Roberts & Rosenthal 2001)
MALA	$d^{-1/3}$	57.4% (Roberts & Rosenthal 2001)
HMC	$d^{-1/4}$	64% (Beskos et. al. 2010)

Extended Parameter Space

- A ball rolling around a surface
- At any time the ball has displacement x and momentum p
- Also has a mass m

The Hamiltonian

$$U(x) = -\log\{\pi(x)\}$$

$$K(p; m) = \frac{1}{2}\frac{p^2}{m}$$

$$H(x, p; m) = U(x) + K(p; m)$$

Hamiltonian Equations

$$\frac{dx}{dt} = \frac{p}{m}$$

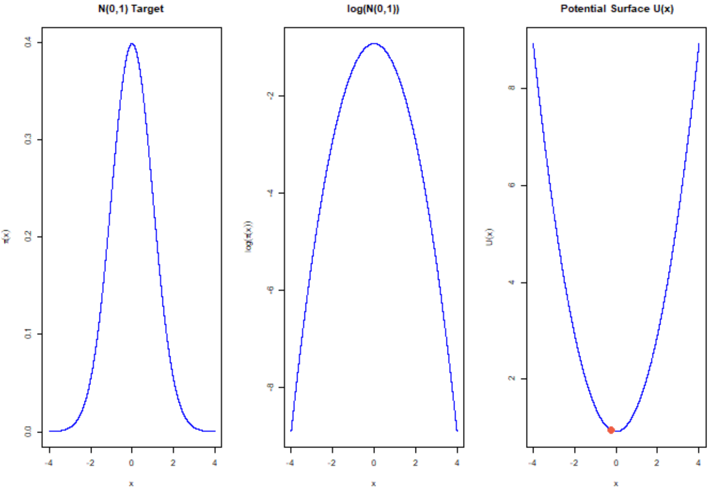
$$\frac{dp}{dt} = -\frac{dU}{dx}$$

Can be generalised to higher dimensions

$$\frac{dx}{dt} = M^{-1}p$$

$$\frac{dp}{dt} = -\nabla U(x)$$

1-dimensional Gaussian Example



Why Hamiltonian Dynamics?

- Reversibility of Hamiltonian Dynamics ensures Detailed Balance.
- If Hamiltonian is conserved, we have acceptance probability of 1
- Volume Preservation

Leapfrog Approximation (Störmer-Verlet)

- A method of approximating Hamiltonian Dynamics
- Preserves the desirable properties of Hamiltonian Dynamics
- Approximately conserves the Hamiltonian
- T, Integration Time
- ε, stepsize
- L, Leapfrog steps

$$T = L\varepsilon \tag{1}$$

HMC Algorithm

- We have some position x.
- Draw a new momentum $p \sim \mathcal{N}(0, M)$.
- Approximate Hamiltonian Dynamics for time T in L steps, using stepsize ε.
- Proposes new position and momentum (x^*, p^*).
- Accept proposal with probability

$$\alpha(x^*, p^*; x, p) = \min\left\{1, \exp(-(H(x^*, p^*; M) - H(x, p; M))\right\}$$

Choosing a Stepsize

- Leapfrog Approximation can become unstable if the chosen stepsize is too large
- On the other hand, if the chosen stepsize is too smaller, the approximation becomes intensive.
- Find a range of stepsizes which perform suitably

Choosing the Integration Time

Optimal Acceptance Rate

Questions

Thank you for listening.

Any Questions?