Hybrid Monte Carlo

Radford M. Neal. An improved acceptance procedure for the hybrid monte carlo algorithm. *J. Comput. Phys.*, 111(1):194–203, 1994

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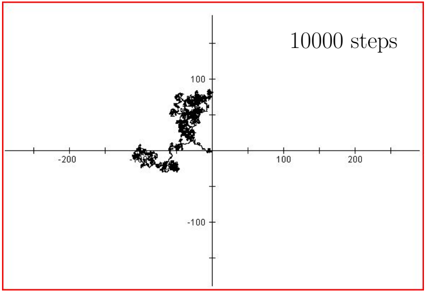
13 Feb 2009

Contents

Current Section

Problem with Naive Metropolis-Hastings

- Random Walks travel expected distance of $O(\sqrt{n})$ after n steps



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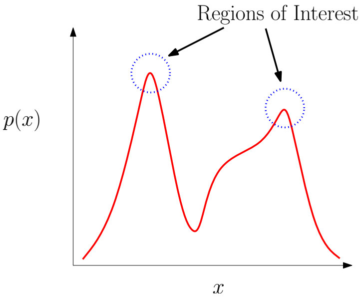
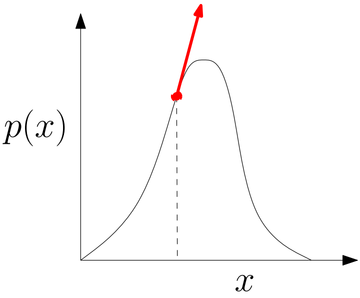


Observation

- When a ball is on an incline, the angle of incline dictates the force with which it rolls down



Characterization for a physical system

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- The gradient of $E(x)$ dictates the change in momentum

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$P(x)$ and $P(u)$ are independent

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- And Then?

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- Modify using above equations to get a new sample

Leapfrog Discretization

$$u(\tau + \frac{\epsilon}{2}) = u(\tau) - \frac{\epsilon}{2} \nabla E(x(\tau))$$

$$x(\tau + \epsilon) = x(\tau) + \epsilon u(\tau + \frac{\epsilon}{2})$$

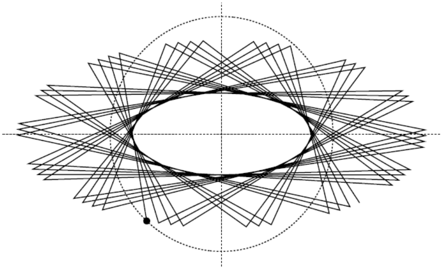
$$u(\tau + \epsilon) = u(\tau + \frac{\epsilon}{2}) - \frac{\epsilon}{2} \nabla E(x(\tau + \epsilon))$$

Time Reversible and Volume Preserving

Current Section

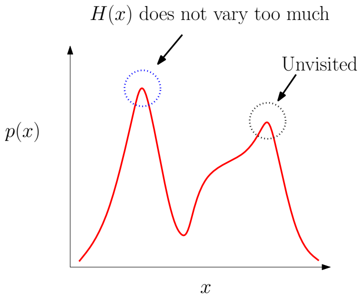
Two problems with the dynamical method

Discretization errors



Two problems with the dynamical method
Energy Well

We might be stuck in an energy well (intuitively, a local maxima)



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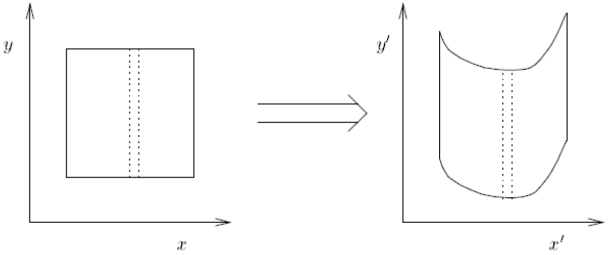
- What does this get us?
  - We can move to regions of different energies H
  - Usually enough to ensure ergodicity

Accept/Reject Step

- Similar to MH
- The Acceptance Probability is a function of the difference in energies

$$a(\Delta H) = min(1, exp(-\Delta H))$$

Detailed Balance



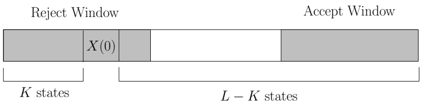
Speed of Computation

- Tunable Parameters - L and ϵ
- Tradeoff between computation time and quality
    - Generally works better for non-local variables (higher dimensions?)

Applications

- Simulation of Physical Systems
- Optimization
- Sampling

Acceptance Procedure using Windows



- Select window to move to
- Select state within window to move to
- Free Energy

$$F(W) = -\log \sum_{X \in W} exp(-H(X))$$

- Acceptance Probability is $a(\Delta F)$

Questions?