

# Hybrid Monte Carlo.

Note Title

5/23/2006

Want to avoid the "random walk" behaviour that is common to Metropolis type algorithm.

Motivated by Physics

Newtonian Physics:

$\underline{x}(t)$   $d$ -dim position vector of particle at time  $t$ .  $\underline{x} = (x_1, \dots, x_d)$   
 $d$ -dim mass vector.  $\underline{m} = (m_1, \dots, m_d)$   
 $\underline{v}(t) \triangleq \dot{\underline{x}}(t)$  is the velocity vector.  
 $\underline{\dot{v}}(t)$  is the acceleration.

$\underline{F} = \underline{m} \underline{\dot{v}}(t)$  Newton's Law of Motion.

Momentum  $\underline{p} = \underline{m} \underline{v}$ .  
 $\underline{m} \underline{v} = (m_1 v_1, \dots, m_d v_d)$

Kinetic Energy  $k(\underline{p}) = \frac{1}{2} \sum_{i=1}^d m_i v_i^2 = \frac{1}{2} \sum_{i=1}^d \frac{p_i^2}{m_i}$

Total energy:  $\mathcal{H}(\underline{x}, \underline{p}) = U(\underline{x}) + k(\underline{p})$

potential energy  $\nearrow$   $\underline{F} = -\underline{\nabla} U(\underline{x})$

## Hamilton's Equations of motion

$$\dot{\underline{x}}(t) = \frac{\partial H(\underline{x}; \underline{p})}{\partial \underline{p}}$$

$$\dot{\underline{p}}(t) = -\frac{\partial H(\underline{x}; \underline{p})}{\partial \underline{x}}$$

Note:

$$\frac{dH}{dt} = \frac{\partial H}{\partial \underline{p}} \cdot \frac{d\underline{p}}{dt} + \frac{\partial H}{\partial \underline{x}} \cdot \frac{d\underline{x}}{dt} = 0$$

Energy is conserved.

Discretize the equations:

Finite Differences:

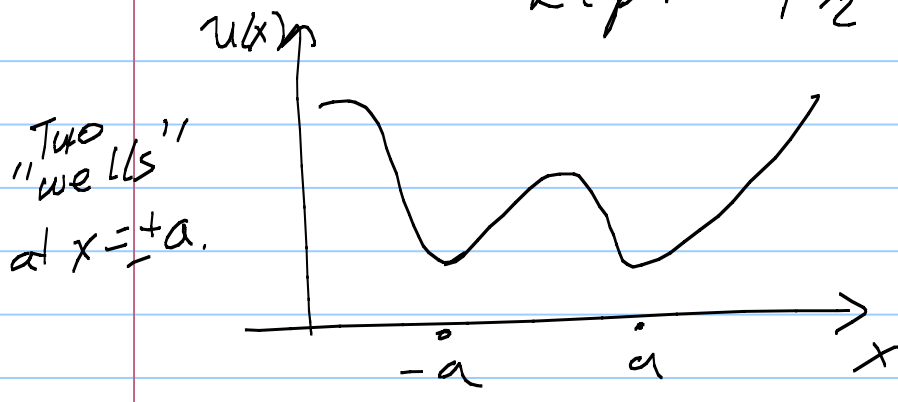
Leap-frog Method:

$$\underline{x}(t+\Delta t) = \underline{x}(t) + \Delta t \cdot \frac{\underline{p}(t+\frac{1}{2}\Delta t)}{m}$$

$$\underline{p}(t+\frac{1}{2}\Delta t) = \underline{p}(t-\frac{1}{2}\Delta t) + \Delta t \cdot \frac{\partial H}{\partial \underline{x}} \Big|_t$$

(Momentum at time  $t$  is  $\frac{1}{2} (\underline{p}(t+\frac{1}{2}\Delta t) + \underline{p}(t-\frac{1}{2}\Delta t))$ )

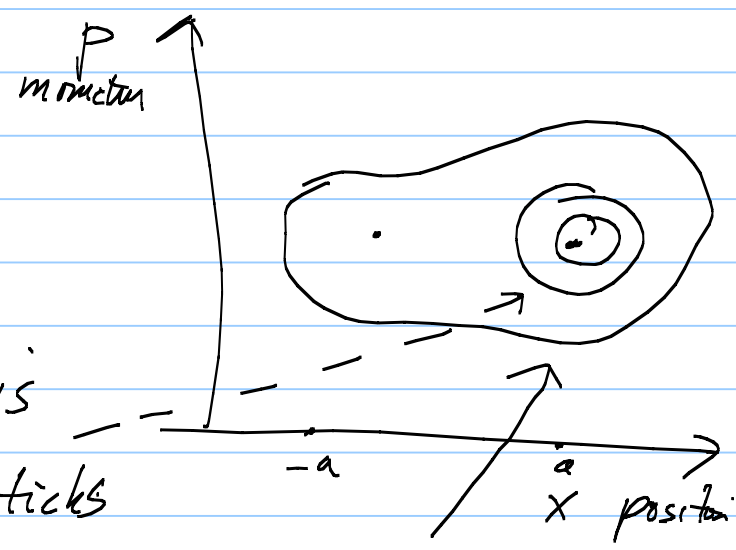
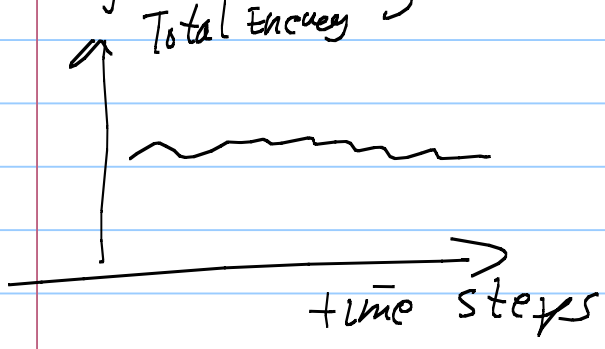
Example:  $u(x) = x^2 + a^2 - \log(\cosh(ax))$   
 $k(p) = p^2/2$



"Two wells"  
at  $x = \pm a$ .

Two minima  
(equal height)  
at  $x = \pm a$ .

After discretization: energy is not conserved.



If initial speed is small, ~~the~~ particle sticks to one well.

If initial speed is big, ~~the~~ particle travels between two wells.

Volume Preservation: In leap-frog, as in exact Hamiltonian Dynamics, the volume is preserved from one step to the next.

Why do we care?

$$\text{Volume } |V(t)| \stackrel{\text{def}}{=} \iint_{V(t)} dx dp.$$

where  $V(t) = \{ (x(t), p(t)) : (x(0), p(0)) \in V(0) \}$

Volume preservation:  $|V(t)| = |V(0)|.$

Intuition for Hybrid Monte Carlo.

The momentum allows the system to escape from local minima.

And the gradient helps guide the system in the right direction.



Hybrid Monte Carlo uses the basic idea of Hamiltonian Systems together with the Metropolis acceptance rule.

Two Basic Observations.

(a) If we can simulate from distribution  $\pi(x, p) \propto e^{-H(x, p)}$  then we can simulate from the marginals  $x \sim \pi(x) \propto e^{-u(x)}$ ,  $p \sim \phi(p) \propto e^{-p^2/m}$ .

(b) The Hamiltonian trajectory is time reversible  $\sim$  relates to volume preserving.

If we run leap-frog from  $(x, p)$  to  $(x', p')$  in  $t$  steps, then we can start from  $(x', -p')$  and run  $t$  steps to get  $(x, -p)$ .

This is needed to ensure reversibility (detailed balance) of the Hybrid Monte Carlo.

## Hybrid Monte Carlo

At time  $t$  and position  $\underline{x}$ .

- Generate a new momentum vector  $\underline{p}$  from the Gaussian  $\phi(\underline{p}) \propto e^{-k(\underline{p})}$ .
- Run the leap-frog algorithm starting from  $(\underline{x}, \underline{p})$  for  $L$  steps, to obtain a new state  $(\underline{x}', \underline{p}')$
- Accept the proposed state  $(\underline{x}', \underline{p}')$  with probability  $\min\{1, \exp\{-H(\underline{x}', \underline{p}') + H(\underline{x}, \underline{p})\}\}$   
Otherwise stay in state  $\underline{x}$ .

$g^L$ -leapfrog

$L$  steps

Why does this work? Heuristic Argument.

(a) Let  $(\underline{x}', \underline{p}') = g^L(\underline{x}, \underline{p})$

$(\underline{x}, -\underline{p}) = g^L(\underline{x}', -\underline{p}')$

(b)  $\pi(\underline{x}, \underline{p}) = \pi(\underline{x}, -\underline{p})$  for any  $\underline{x}, \underline{p}$

(c) By volume preservation  $d\underline{x} d\underline{p} = d\underline{x}' d\underline{p}'$   
suggests the proposal is symmetric (as required by Metropolis). More rigorous proof in Liu.