Monte Carlo methods in Artificial Intelligence and Machine Learning

Hybird Monte Carlo

Chun Yuan, BR Sameh, Yang Chen

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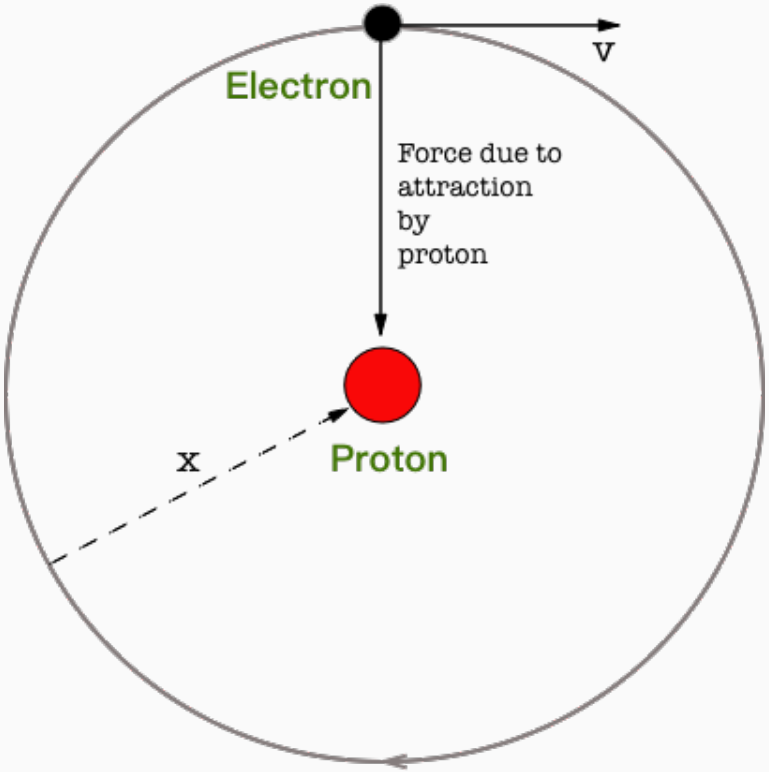
Overview

1. Background Knowledges
2. Hamiltonian System
3. Hamiltonian Monte Carlo(HMC)
   Hybrid
4. Comparison with Random Walk and Langevin Sampling
5. Conclusion

Background Knowledges

Conservation of mechanical energy

For an isolated system, its mechanical energy remains constant in time.[1]

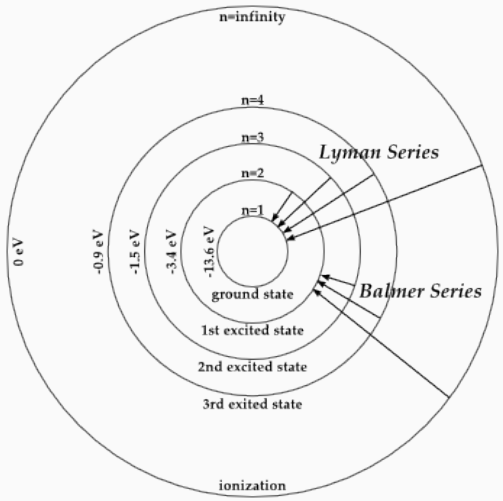


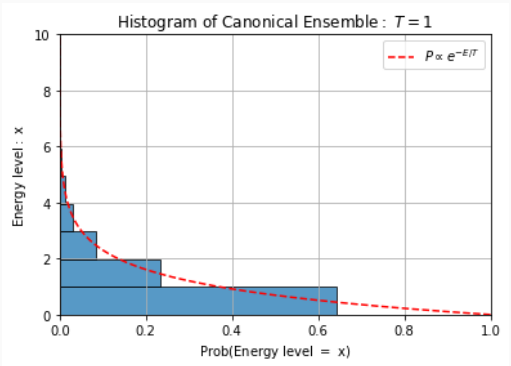
$$E(x, v) = U(x) + K(v) = const.$$

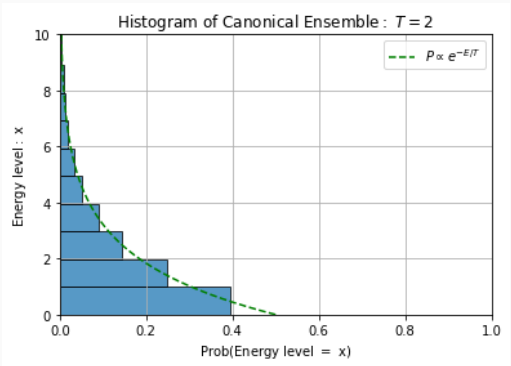
$U(x)$ is potential energy
$K(v)$ is kinetic energy

Canonical Ensemble

In statistical mechanics, the **canonical ensemble** is the statistical ensemble that represents **the possible states** of a mechanical system at a **fixed** temperature.[2]

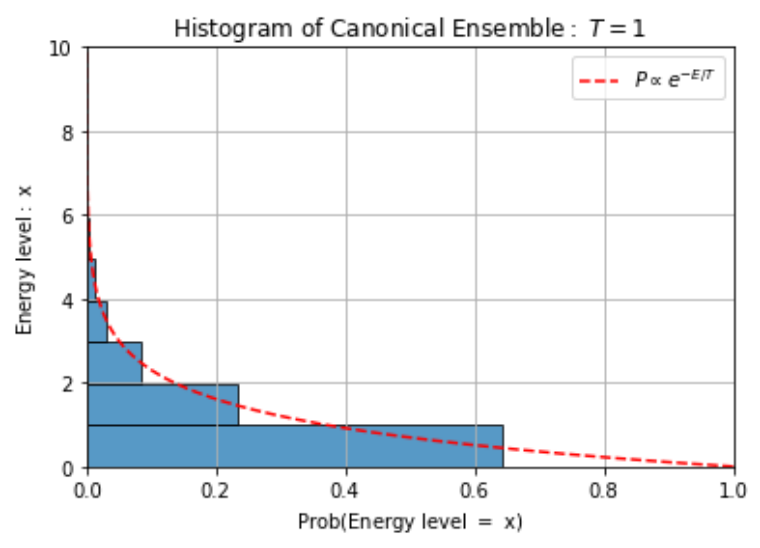






Canonical Ensemble

The histogram below describes the amount of hydrogen's electrons which stay at different possible energy levels. The canonical ensemble could be defined as:



$$\Pi(x, v) = \frac{1}{Z} e^{-\frac{E(x,v)}{T}} = \frac{1}{Z} e^{-\frac{U(x)+K(v)}{T}}$$

E is electron's mechanical energy

T is surrounding temperature

Z is the normalisation part

Hamiltonian System

Background of Hamiltonian System

A Hamiltonian system is a dynamical system governed by Hamilton's equations. In physics, this dynamical system describes the evolution of a physical system such as a planetary system or an electron in an electromagnetic field.[3]

Energies in Hamiltonian system also follows the conversation of mechanical energy, and could be represented as canonical ensemble as following:

$$H(x, v) \propto e^{-\frac{U(x)+K(v)}{T}} = const.$$

where, $\underline{x}$ indicates the position information and $\underline{v}$ is the velocity.

System Dynamics

Random walk sampler utilizes:

$$\underline{x}(t+\epsilon) = \underline{x}(t) + \sqrt{\rho}\underline{z}$$

where $z \sim \mathcal{N}(0, \underline{I})$

Langevin sampling adds some extra information(gradient information) into the dynamics:

$$\underline{x}(t+\epsilon) = \underline{x}(t) + \frac{\epsilon}{2}\nabla \ln p(\underline{x}(t)) + \eta\sqrt{\epsilon}$$

Hamiltonian Equations

In Hamiltonian Monte Carlo, in order to sampling from the joint density, we make use of Hamiltonian Equations:

$$\frac{dp}{dt} = -\frac{\partial H}{\partial x}$$

$$\frac{dx}{dt} = +\frac{\partial H}{\partial p}$$

Simple explanation:[4]

- The first Hamilton equation means that the force equals the negative gradient of potential energy.
- The second Hamilton equation means that the particles velocity equals the derivative of its kinetic energy with respect to its momentum.

Numerical Methods for Hamiltonian Equations

Hamiltonian equations are two differential equations. Therefore, to update our position information $\underline{x}$ and momentum $\underline{p}$, we need methods to compute these differential equation. There exist various algorithm to achieve this:

- Euler's method
- Euler's modified method
- Leapfrog method

Numerical Methods for Differential Equations

- Euler's Method:

If we start at t = 0 with given values for x(0) and p(0), we can iterate the steps above to get a trajectory of position and momentum values at times ε, 2ε, 3ε, . . .,

$$\begin{cases} p(t+\epsilon) = p(t) + \epsilon \frac{dp}{dt}(t) = p(t) - \epsilon \frac{\partial H}{\partial x}|_{x(t)} \\ x(t+\epsilon) = x(t) + \epsilon \frac{dx}{dt}(t) = x(t) + \epsilon \frac{\partial H}{\partial p}|_{p(t)} \end{cases}$$

- Euler's Modified Method:

We simply use the new value for the momentum variables p, when computing the new value for the position variables, x. A method with similar performance can be obtained by instead updating the x first and using their new values to update the p

$$\begin{cases} p(t+\epsilon) = p(t) - \epsilon \frac{\partial H}{\partial x}|_{x(t)} \\ x(t+\epsilon) = x(t) + \epsilon p(t+\epsilon) \end{cases}$$

- Leapfrog Method:

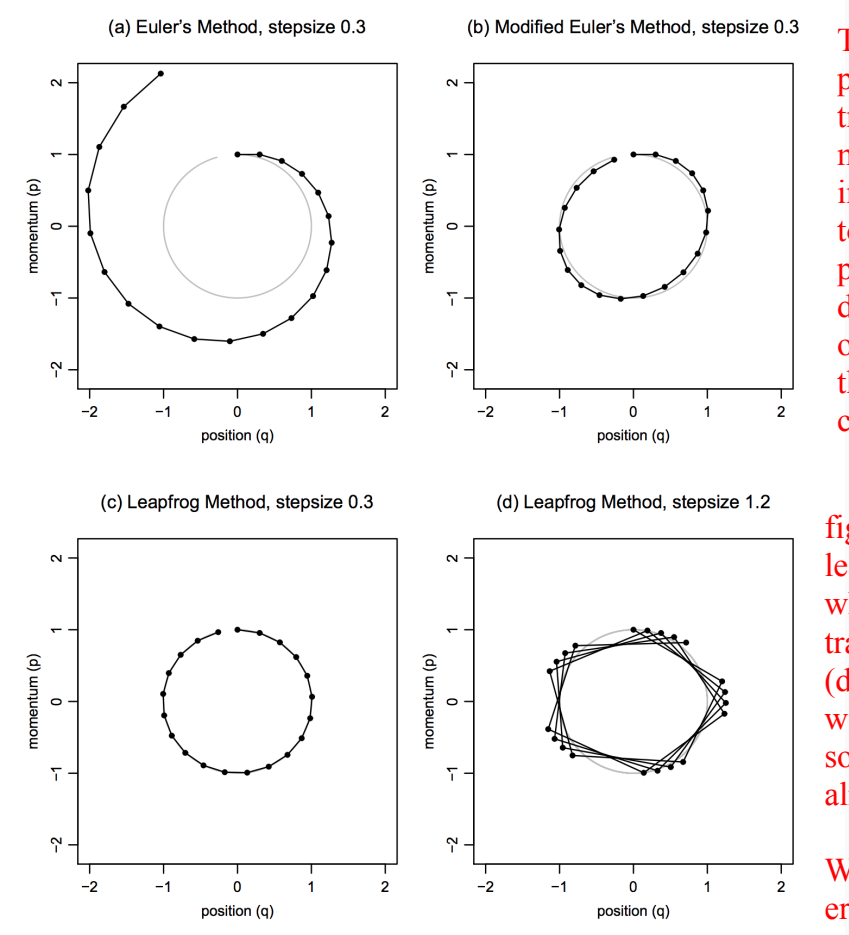
The leapfrog method then looks very similar to the modification of Euler's method except that leapfrog performs half steps for momentum at the very beginning and very end of the trajectory, and the time labels of the momentum values computed are shifted by ε/2.

$$\begin{cases} p(t+\frac{\epsilon}{2}) = p(t) - \frac{\epsilon}{2} \frac{\partial H}{\partial x}|_{x(t)} \\ x(t+\epsilon) = x(t) + \epsilon p(t+\frac{\epsilon}{2}) \\ p(t+\epsilon) = p(t+\frac{\epsilon}{2}) - \frac{\epsilon}{2} \frac{\partial H}{\partial x}|_{x(t+\epsilon)} \end{cases}$$

We start with a half step for the momentum variables, then do a full step for the position variables, using the new values of the momentum variables, and finally do another half step for the momentum variables, using the new values for the position variables.

The results using three methods for approximating Hamiltonian dynamics: [5](section 3.2)

Euler's method produces a trajectory that diverges to infinity, but the true trajectory is a circle.



Though not perfect, the trajectory it produces is much closer to the true trajectory than that obtained using Euler's method, with no tendency to diverge to infinity. This better performance is related to the modified method's exact preservation of volume, which helps avoid divergence to infinity or spiraling into the origin, since these would typically involve the volume expanding to infinity or contracting to zero.

figure (c) shows the results using the leapfrog method with a stepsize of $\varepsilon = 0.3$, which are indistinguishable from the true trajectory, at the scale of this plot. In Figure (d), the results of using the leapfrog method with $\varepsilon = 1.2$ are shown (still with 20 steps, so almost four cycles are seen, rather than almost one).

With this larger stepsize, the approximation error is clearly visible, but the trajectory still remains stable (and will stay stable indefinitely). Only when the stepsize approaches $\varepsilon = 2$ do the trajectories become unstable.

Local and Global Error of Discretization Methods

It's easy to get:

$$\lim_{\epsilon \to 0} \mathcal{E}_{Approx} = 0$$

Therefore, we have to apply upper bound to the error function.

We define:

- The local error is the error after one step;
- The global error is the error after simulating for some fixed time interval s.

If the local error is order ϵ^a, in this time interval s, frog will jump s/ϵ steps:

$$O(\mathcal{E}_g) = O(\mathcal{E}_{loc}) * \frac{s}{\epsilon} = O(\epsilon^{a-1})$$

As shown by Neal (2011, section 2.3), The Euler method and its modication above have order ϵ^2 local error and order ϵ global error. The leapfrog method has order ϵ^3 local error and order ϵ^2 global error.[5]

So far ...

- The joint distribution of the system energies could be formulated as:

$$\Pi(x, p) = e^{-\frac{U(x)+K(p)}{T}}$$

- System's dynamics:

$$\begin{cases} p(t+\frac{\epsilon}{2}) = p(t) - \frac{\epsilon}{2}\frac{\partial H}{\partial x}|_{x(t)} \\ x(t+\epsilon) = x(t) + \epsilon p(t+\frac{\epsilon}{2}) \\ p(t+\epsilon) = p(t+\frac{\epsilon}{2}) - \frac{\epsilon}{2}\frac{\partial H}{\partial x}|_{x(t+\epsilon)} \end{cases}$$

- our goal is: to obtain samples x from the joint distribution $\underline{\Pi(x, p)}$ regardless of samples $\underline{p}$

Hamiltonian Monte Carlo(HMC)

Hybrid

Basic Assumptions in HMC

Assumed that system's potential energy is $\underline{U(x) = -\log \pi(x)}$ and kinetic energy has the form $\underline{K(p) = \frac{p^2}{2m}}$.

Then, the canonical ensemble for this system is:

$$\Pi(x, p) = e^{-\frac{U(x)+K(p)}{T}} \propto \pi(x) e^{-\frac{p^2}{2mT}} \doteq \pi(x)\pi'(p)$$

This indicates that $\underline{x}$ and $\underline{p}$ are **independent** with each other.

Basic Assumptions in HMC

Since the kinetic energy could be represented as:

$$\pi'(p) = e^{-\frac{p^2}{2mT}}$$

which is similar with a Gaussian density with zero mean and unit variance.

Therefore, we suppose that the distribution of kinetic energy is:

$$\pi'(p) \sim \mathcal{N}(0, 1)$$

Metropolis-Hastings Algorithm in HMC

The acceptance ratio of Metropolis-Hastings method in MCMC is:

$$A(x'|x) = \min \left\{ \frac{p(x')q(x|x')}{p(x)q(x'|x)} \ , \ 1 \right\}$$

where $q(\cdot)$ is a proposal distribution.

Hybrid

In Hamiltonian Monte Carlo, the canonical ensemble of system energies is the corresponding proposal distribution: $\Pi(x,p) = \pi(x)\pi'(p)$. Hence, the acceptance ratio for HMC is:

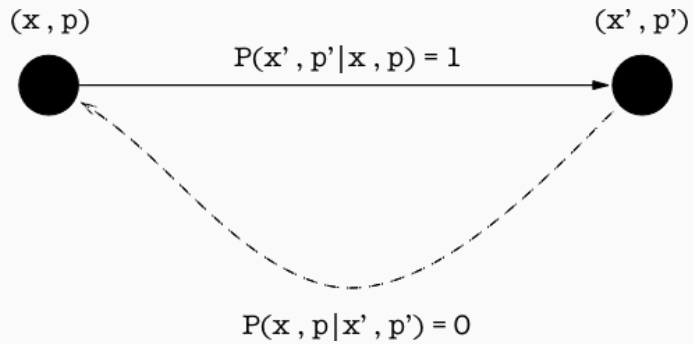
$$A(x',p'|x,p) = \min \left\{ \frac{\Pi(x',p')}{\Pi(x,p)} \frac{p(p,x|p',x')}{p(p',x'|p,x)} \ , \ 1 \right\}$$

Metropolis-Hastings Algorithm in HMC

- The first term is the ratio of proposals, more specifically, it is just the difference of system energies in two different states:

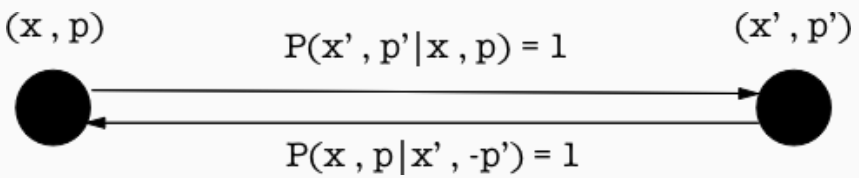
$$\frac{\Pi(x', p')}{\Pi(x, p)} = exp\{-\frac{E_{new} - E_{old}}{T}\}$$

- The second term is about the path of particle. However, it is deterministic, according to our system dynamics.In this case, the acceptance ratio will decrease to $\underline{0}$.



The Negation of Momentum

Instead of choosing proposal (x', p'), we first flip the direction of momentum p' to $-p'$, and select $(x', -p')$ as our proposal.



This operation will lead the second term $\frac{p(p,x|p',x')}{p(p',x'|p,x)} = 1$

This negation of momentum need not be done in practice, since $K(p) = K(-p)$.[5]

Acceptance of new Proposal in HMC

Now, the acceptance ratio for Hamiltonian Monte Carlo could be simplified as:

Hybrid

$$A(x', p'|x, p) = \min\left\{ \frac{\Pi(x', p')}{\Pi(x, p)} \ , \ 1 \right\} = \min\left\{ exp^{-\frac{E_{new} - E_{old}}{T}} \ , \ 1 \right\}$$

Algorithm 1: Accept New Proposal

input : Initial State: (x_t, p_t)

output: New Proposal: (x_{t+1}, p_{t+1})

$A(x_{t+1}, p_{t+1}|x_t, p_t) = exp\{\frac{E_{old} - E_{new}}{T}\}$;

if $A(x_{t+1}, p_{t+1}|x_t, p_t) >= u \sim U(0, 1)$ **then**

  $s = x_{t+1}$;

else

  $s = x_t$;

end

Hamiltonian Monte Carlo Sampling

Hybrid

There exits two steps in the HMC sampling at each iteration:[5](section 3.2)

- The first step: new values for the momentum variables are randomly drawn from their Gaussian distribution, independently of the current values of the position variables.

- In the second step, a Metropolis update is performed, using Hamiltonian dynamics to propose a new state.

Note: the momentum will be replaced before it is used again, in the rst step of the next iteration. Therefore, we don't have to inverse its direction.

Hamiltonian Monte Carlo Sampling

Hybrid

Algorithm 2: Hamiltonian Monte Carlo Sampling

Hybrid

input : The Number of Samples: N, Step Size: ϵ, System Temperature: T

output: Samples: $\underline{X} = (x_1, ..., x_n)$ from $p(x)$

initialization: choose x_t randomly, $t = 1$;
while $t < N$ **do**
    each time choose p_t randomly;
    $(x_{t+1}, p_{t+1}) = leapfrog(x_t, p_t, steps, \epsilon)$;
    if $A(x_{t+1}, p_{t+1}|x_t, p_t) >= u \sim U(0, 1)$ **then**
        $s = x_{t+1}$;
    else
        $s = x_t$;
    end
    Appending s to $\underline{X}$;
    t+=1;
end

Comparison with Random Walk and Langevin Sampling

Bases for the first Experiment

Experiment 1: Given two-dimensional Gaussian distribution with mean vector $\underline{\mu} = (0, 0)^T$ and covariance matrix $\underline{\Sigma} = \begin{pmatrix} 1.0 & 0.6 \\ 0.6 & 2.0 \end{pmatrix}$.

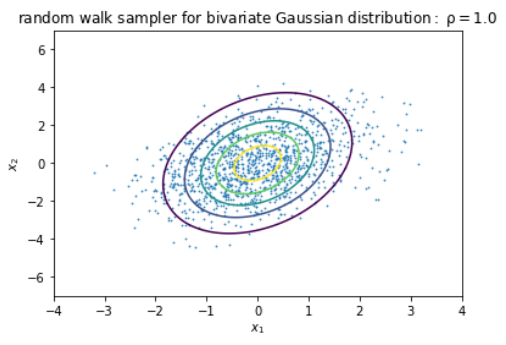
We apply respectively Random Walk, Langevin and Hybird Monte Carlo sampling methods to generate $N = 2000$ samples, and calculate their corresponding covariance matrices with various hyperparameters.

sample n=2000 times

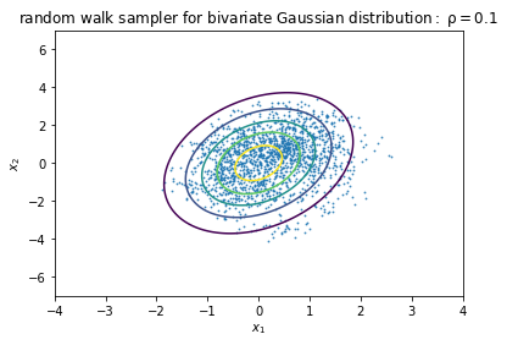
parameters

Random Walk Sampling

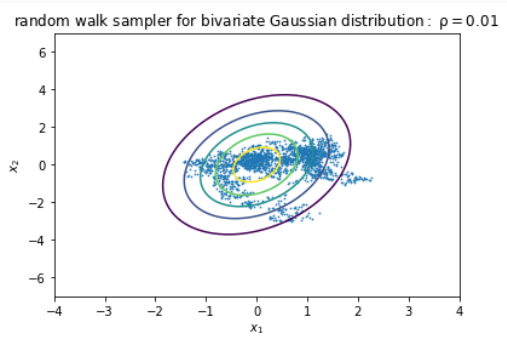
The dynamics of Random Walk Sampling is: $\underline{x}' = \underline{x} + \sqrt{\rho}\underline{z}$



(a) rho: 1.0



(b) rho: 0.1



(c) rho: 0.01

$$\begin{pmatrix} 1.07 & 0.63 \\ 0.63 & 2.22 \end{pmatrix}$$

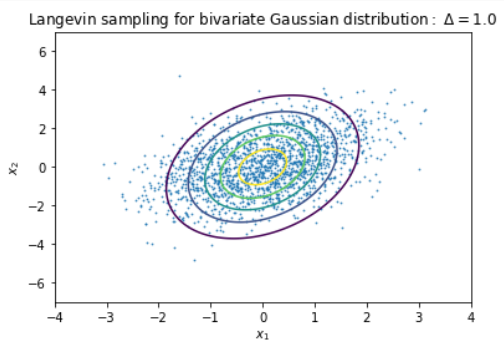
$$\begin{pmatrix} 0.91 & 0.76 \\ 0.76 & 2.10 \end{pmatrix}$$

$$\begin{pmatrix} 0.56 & 0.77 \\ 0.77 & 2.91 \end{pmatrix}$$

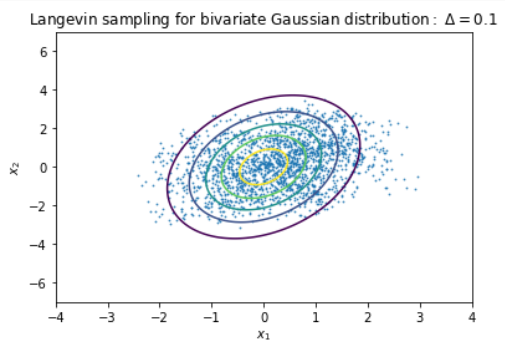
Langevin Sampling

The dynamics of Langevin Sampling is:

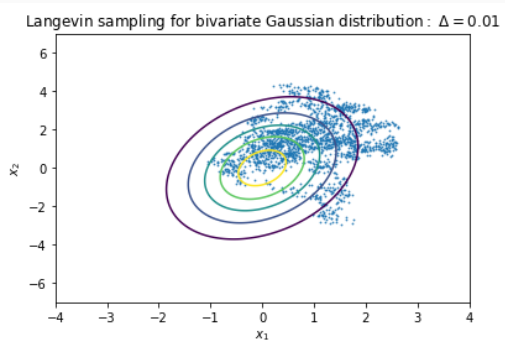
$$\underline{x}(t+\Delta) = \underline{x}(t) + \frac{1}{2}\nabla \ln p(\underline{x}(t))\Delta + \eta\sqrt{\Delta}$$



(a) delta: 1.0



(b) delta: 0.1



(c) delta: 0.01

$$\begin{pmatrix} 1.02 & 0.61 \\ 0.61 & 1.99 \end{pmatrix}$$

$$\begin{pmatrix} 0.99 & 0.55 \\ 0.55 & 2.26 \end{pmatrix}$$

$$\begin{pmatrix} 1.19 & 0.13 \\ 0.13 & 0.97 \end{pmatrix}$$

Hamiltonian Monte Carlo Sampling

Hybrid

The dynamics of HMC Sampling is:

$$\begin{cases} \frac{dp}{dt} = -\frac{\partial H}{\partial x} \\ \frac{dx}{dt} = +\frac{\partial H}{\partial p} \end{cases}$$

There are several parameters in Hamiltonian Monte Carlo sampling which we can play with:

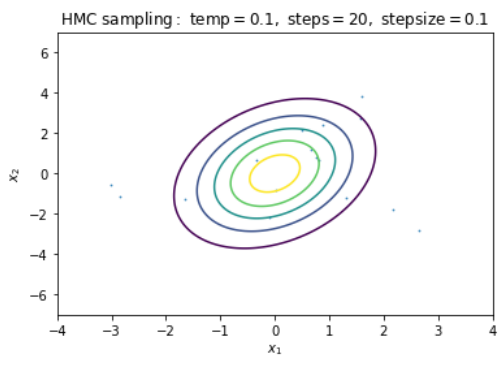
Hybrid

The system temperature: $\underline{T}$, the number of jumping step for leap frog: $\underline{N}$, and the size of jumping step: $\underline{\epsilon}$.

Hamiltonian Monte Carlo Sampling

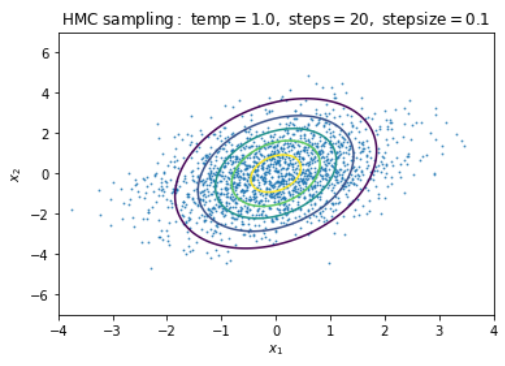
Hybrid

Let the system temperature change only:



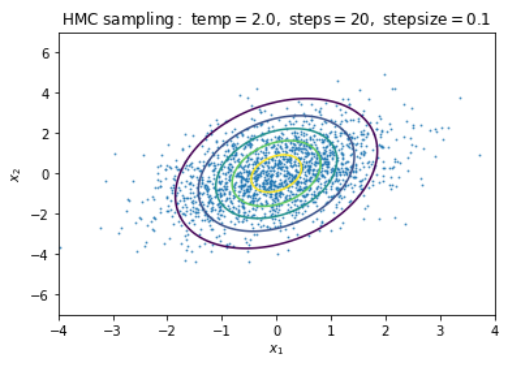
(a) temperature: 0.1

$$\begin{pmatrix} 2.57 & 0.61 \\ 0.61 & 3.51 \end{pmatrix}$$



(b) temperature: 1

$$\begin{pmatrix} 1.15 & 0.57 \\ 0.57 & 2.17 \end{pmatrix}$$



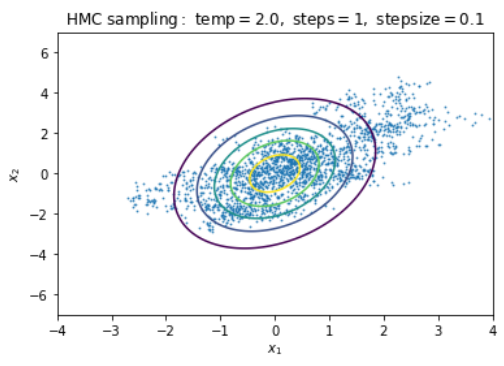
(c) temperature: 2

$$\begin{pmatrix} 1.06 & 0.60 \\ 0.60 & 2.02 \end{pmatrix}$$

Hamiltonian Monte Carlo Sampling

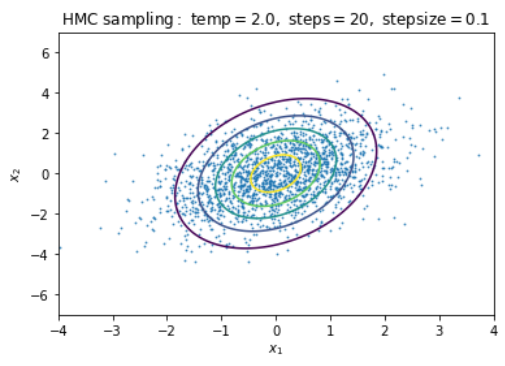
Hybrid

Let the frog's jumping steps change only:



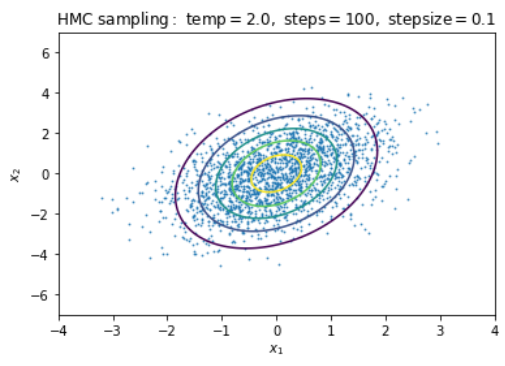
(a) steps: 1

$$\begin{pmatrix} 1.46 & 1.34 \\ 1.34 & 2.29 \end{pmatrix}$$



(b) steps: 20

$$\begin{pmatrix} 1.15 & 0.57 \\ 0.57 & 2.17 \end{pmatrix}$$



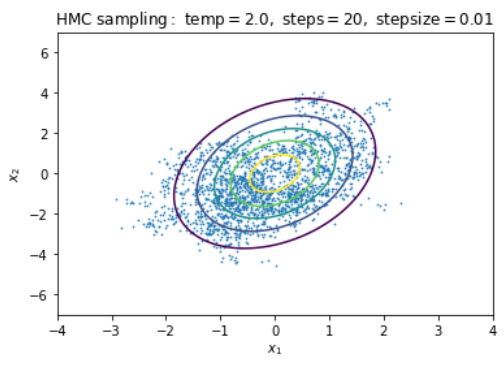
(c) steps: 100

$$\begin{pmatrix} 0.95 & 0.66 \\ 0.66 & 2.20 \end{pmatrix}$$

Hamiltonian Monte Carlo Sampling

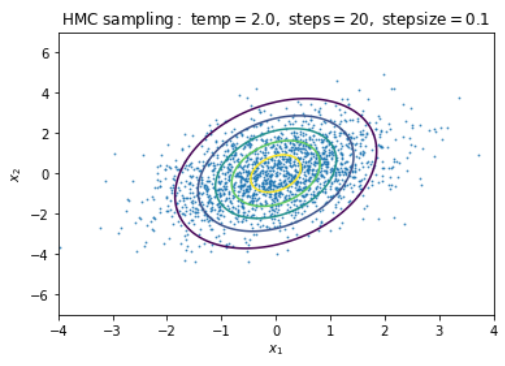
Hybrid

Let the size of jumping change only:



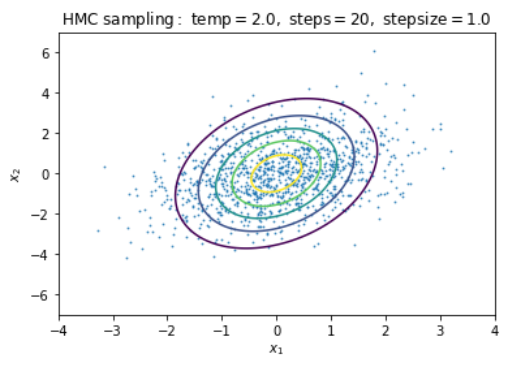
(a) epsilon: 0.01

$$\begin{pmatrix} 0.99 & 0.79 \\ 0.79 & 2.58 \end{pmatrix}$$



(b) epsilon: 0.1

$$\begin{pmatrix} 1.15 & 0.57 \\ 0.57 & 2.17 \end{pmatrix}$$



(c) epsilon: 1.0

replace

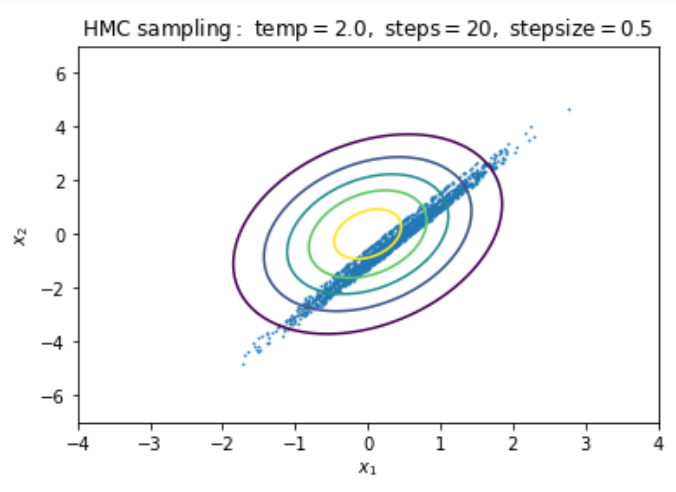
$$\begin{pmatrix} 1.17 & 0.58 \\ 0.58 & 2.12 \end{pmatrix}$$

Ergodicity of Hamiltonian Monte Carlo

Hybrid

Typically, the HMC algorithm will not be trapped in some subset of the state space, and hence will asymptotically converge to its invariant distribution.

However, ergodicity can fail if the L leapfrog steps in a trajectory produce an exact periodicity for some function of state.[5]



Here is an instance we met

This potential problem can be solved by randomly choosing ϵ or L (or both) from some fairly small interval.[6]

Bases for the second Experiment

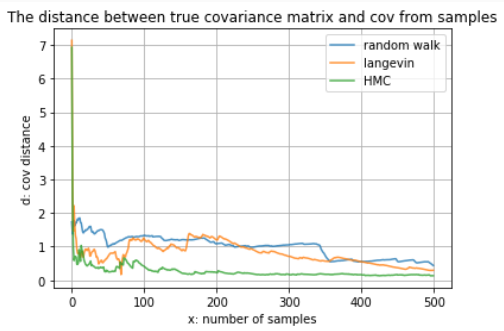
Experiment 2: The same with the first one, given two-dimensional Gaussian distribution with mean vector $\underline{\mu} = (0, 0)^T$ and covariance matrix $\underline{\Sigma} = \begin{pmatrix} 1.0 & 0.6 \\ 0.6 & 2.0 \end{pmatrix}$.

We apply respectively Random Walk, Langevin and Hybird Monte Carlo sampling methods to obtain the same amount of accepted samples, and calculate the distance between their corresponding covariance matrices and the true one.

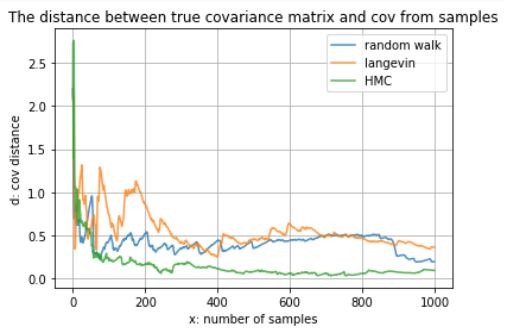
Hamiltonian Monte Carlo Sampling

Hybrid

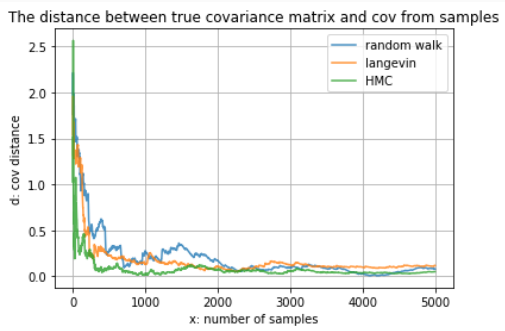
Utilizing Frobenius matrix norm:



(a) Accepted: 500



(b) Accepted: 1000



(c) Accepted: 5000

Bases for the third Experiment

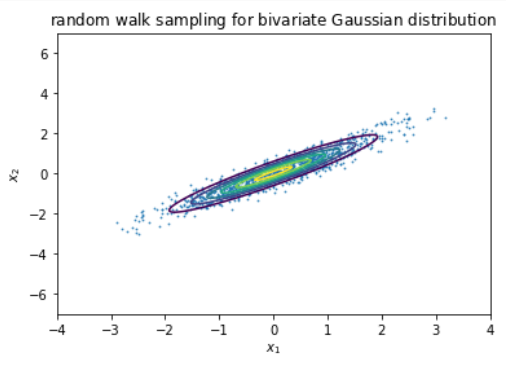
Experiment 3: Given two-dimensional Gaussian distribution with mean vector $\underline{\mu} = (0, 0)^T$ and covariance matrix $\underline{\Sigma} = \begin{pmatrix} 1.0 & 0.95 \\ 0.95 & 1.0 \end{pmatrix}$.

We apply respectively Random Walk, Langevin and Hybird Monte Carlo methods to sample 5000 times, and compare the amount of accepted samples, in order to prove the high efficiency of HMC.

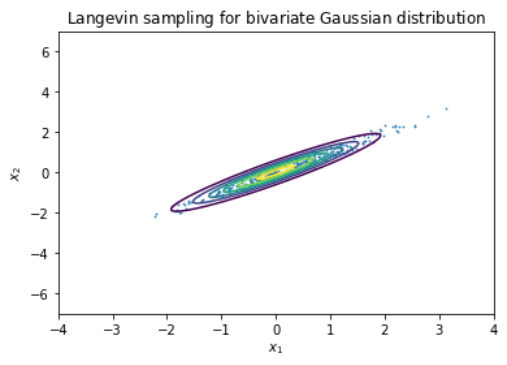
Hamiltonian Monte Carlo Sampling

Hybrid

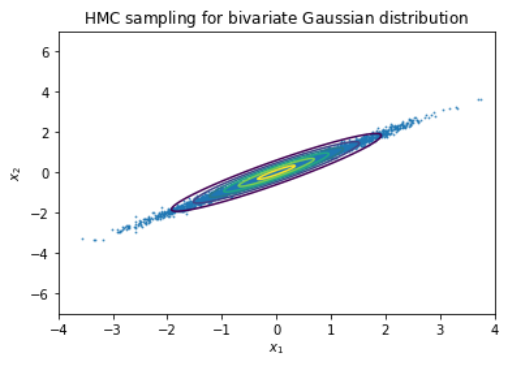
With difference amount of accepted samples:



(a) Accepted: 1206



(b) Accepted: 326



(c) Accepted: 4799

HMC and Its Benefits

Experiment 3 is a nice example to show the advantages of HMC sampling, comparing with the other two methods.
There is also an illustration shown by Neal (2011, section 3.3)[5]:

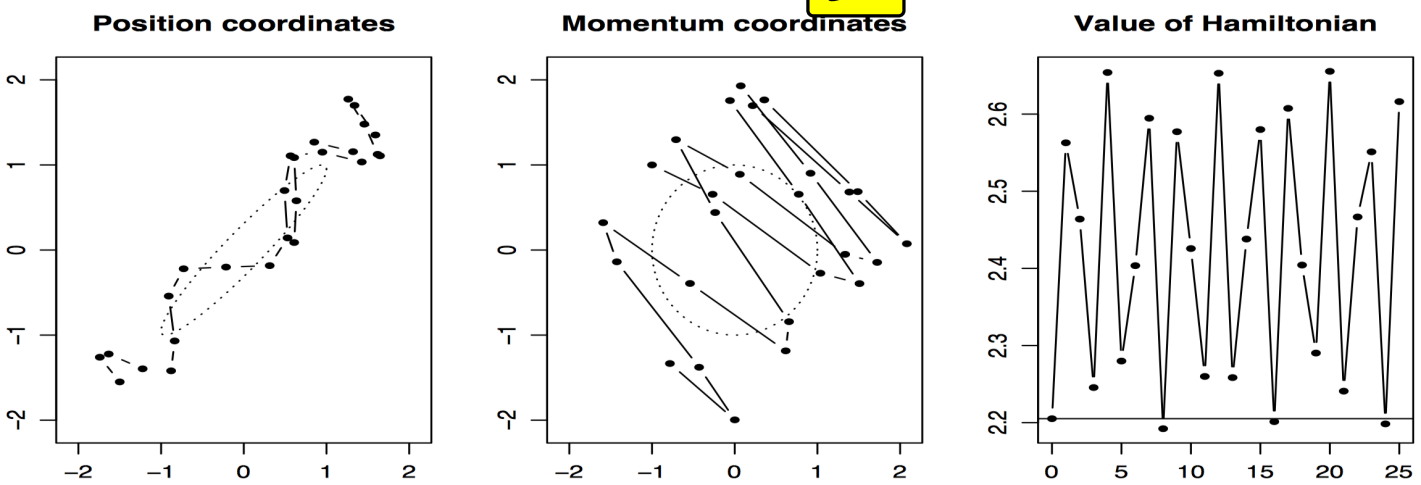


Figure 3: A trajectory for a 2D Gaussian distribution, simulated using 25 leapfrog steps with a stepsize of 0.25. The ellipses plotted are one standard deviation from the means. The initial state had $q = [-1.50, -1.55]^T$ and $p = [-1, 1]^T$.

HMC and Its Benefits

Avoidance of random-walk behaviour, as illustrated above, is one major benet of Hamiltonian Monte Carlo.[5]

Hybrid

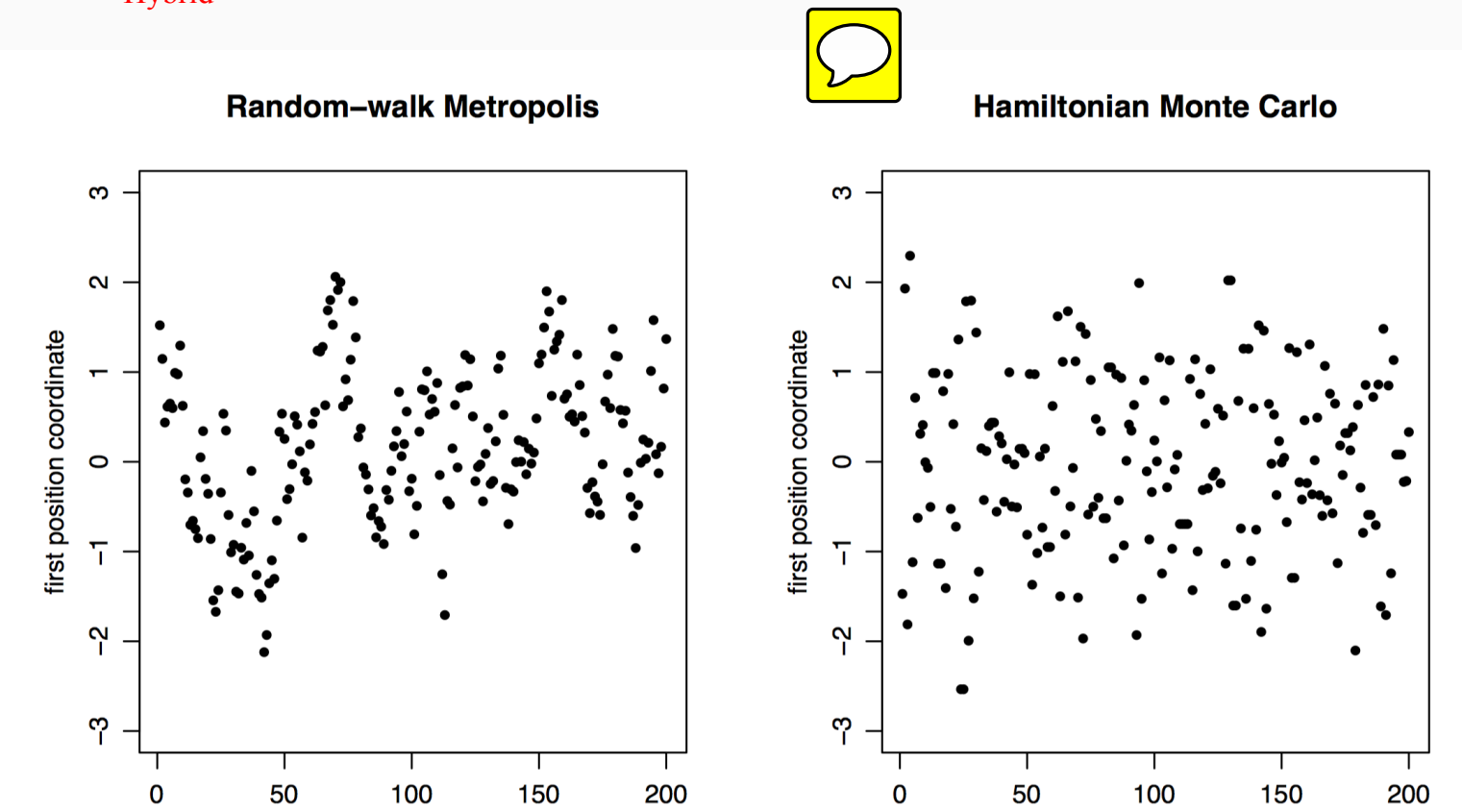


Figure 5: Two hundred iterations, starting with the twenty iterations shown above, with only the first position coordinate plotted.

Taking One Step at A Time: The Langevin Method

If we express an iteration of HMC with one leapfrog step in the following way:

$$\begin{cases} x(t+\epsilon) = x(t) - \frac{\epsilon^2}{2}\frac{\partial H}{\partial x}|_{x(t)} + \epsilon p(t) \\ p(t+\epsilon) = p(t) - \frac{\epsilon}{2}\frac{\partial H}{\partial x}|_{x(t)} - \frac{\epsilon}{2}\frac{\partial H}{\partial x}|_{x(t+\epsilon)} \end{cases}$$

Again we sample the momentum p from their Gaussian distribution with zero mean and unit variance.
Besides, we accept x as the new state with probability:

$$min\{1, exp(-(U(x(t+\epsilon) - U(x)) - \frac{1}{2}(x^2(t+\epsilon) - x^2(t))))\}$$

The equation for x update is known in physics as one type of "Langevin equation", and it is a special case of Hamiltonian Monte Carlo.[7]

Hybrid

Another Way to Avoid Random Walks

Although LMC can be seen as a special case of HMC, it will explore the distribution via an inefficient random walk, just like random-walk Metropolis updates.

However, there is another way to keep it away from randomly walking, that is, so called "partial momentum refreshment", as proposed by Horowitz (1991)[8].

The main idea is a linear combination between the previous momentum state and a random noise, which has the same mean and covariance matrix with the distribution of momentum:

$$p(t+\epsilon) = \alpha p(t) + \sqrt{(1-\alpha^2)}n, \qquad \textit{where } \alpha \in [-1,1] \;\; \textit{and} \;\; n \sim \mathcal{N}(0, I)$$

Conclusion

Potential Problem in Hamiltonian Monte Carlo Sampling

Hybrid

Potential Problem:

- System energy may not be conserved

To reduce this negative influence, we have employed two tricks:

- Leapfrog numerical integration, which is reversible in time
- Metropolis-Hastings rejections to compensate difference in energy between energy at the start and in the end

Pros and Cons of Hamiltonian Monte Carlo

Cons:

Hybrid

- Hamiltonian Monte Carlo accepts in most cases new states
- Less iterations to get representative sampling

Pros:

- The gradient of desired distribution $p(x)$ may not exist
- The computational time of gradient may last a long time
- Problems with sampling from distributions with isolated local minimums(*Tempering during a trajectory*)

The most symmetrical scheme is to multiply the momentum by α before the first half-step for momentum and after the second half-step for momentum, for leapfrog steps in the first half of the trajectory, and correspondingly, to divide the momentum by α before the first and after the second half-steps for momentum in the second half of the trajectory.

Questions?

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