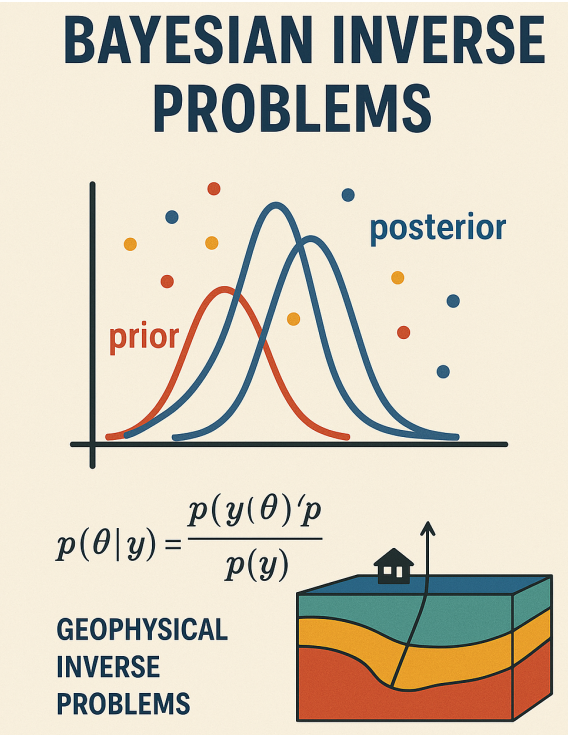
Posterior Estimation Practical: MC, McMC, HMC, V.I.

Mark Asch - MAKUTU/2025



MONTE CARLO

Recall: Monte Carlo Integration

Algorithm

1. Simulate uniform random variables $X_1, X_2, \ldots, X_n$ which can be done using software generated $U_1, U_2, \ldots, U_n$ independent and identically distributed (i.i.d.) uniform random variables on $[0, 1]$.

2. Then let $X_i = a + (b - a)U_i$ for $i = 1, 2, \ldots, n$. Thus, $X_1, X_2, \ldots, X_n$ are independent and identically distributed uniform random variables on $[a, b]$.

3. Evaluate $f(X_1), f(X_2), \ldots, f(X_n)$.

4. Take the average of $f(X_1), f(X_2), \ldots, f(X_n)$ by computing

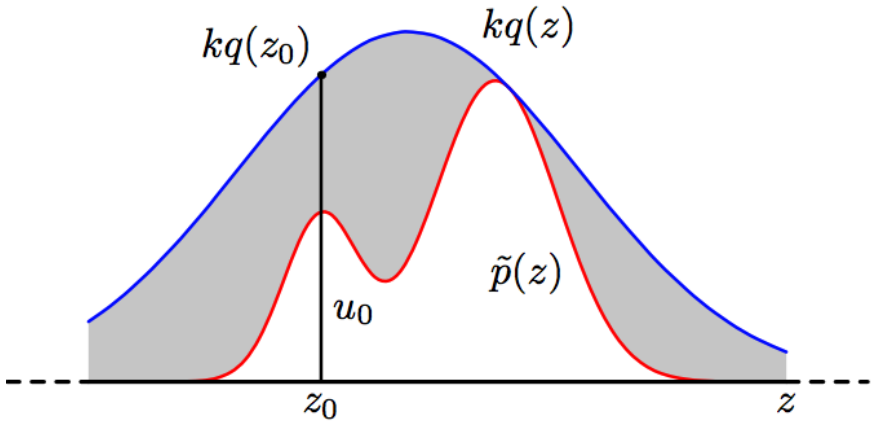
$$(b-a)\frac{1}{n}\sum_{i=1}^{n} f(X_i) = (b-a)\frac{f(X_1)+f(X_2)+\cdots+f(X_n)}{n}$$

and then by the strong law of large numbers this converges to

$$\begin{aligned}(b-a)\,\mathrm{E}(f(X_1)) &= (b-a)\int_a^b f(x)\frac{1}{b-a}\,\mathrm{d}x \\ &= \int_a^b f(x)\,\mathrm{d}x\end{aligned}$$

Recall: Monte Carlo Integration

Sampling Strategies: Rejection Sampling



- **Algorithm**:

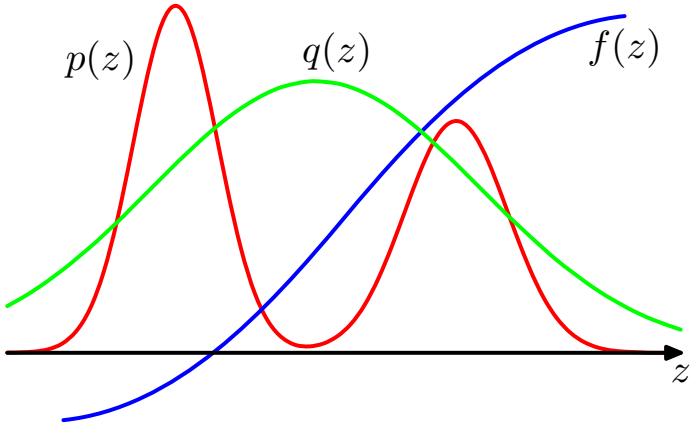
  $\Rightarrow$ Define a simple distribution $q(z)$ and find a k such that for all z

$$kq(z) \geq \tilde{p}(z).$$

  $\Rightarrow$ Draw $z_0 \sim q(z)$.
  $\Rightarrow$ Draw $u_0 \sim \mathcal{U}\left[0, kq(z_0)\right]$.
  $\Rightarrow$ Discard if $u_0 > \tilde{p}(z_0)$, otherwise retain u_0.

Recall: Monte Carlo Integration

Sampling Strategies: Importance Sampling



Input:

- Target distribution $p(x)$, Function of interest $f(x)$, Proposal distribution $q(x)$, Number of samples N

1. **Initialize**: Set sum $S = 0$
2. **For** $i = 1$ to N:
   (a) **Sample**: Generate $x_i \sim q(x)$

(b) **Compute weight** : $w_i = \frac{p(x_i)}{q(x_i)}$
(c) **Evaluate**: $y_i = f(x_i) \cdot w_i$
(d) **Accumulate**: $S = S + y_i$

3. **Estimate**: $\hat{\mu}_{\mathrm{IS}} = \frac{S}{N}$

Ex. 1: Monte Carlo Integration

Estimate π

This is a well-known, introductory exercise in Monte Carlo integration. Compute the area under the first quadrant of the unit circle, where the function to integrate is

$$f(x,y) = \begin{cases} 1 & \text{for } x^2 + y^2 \leq 1, \\ 0 & \text{otherwise,} \end{cases}$$

and the integral

$$I = \int_0^1 \int_0^1 f(x,y)\,\mathrm{d}x\mathrm{d}y.$$

Then $I \approx \pi/4$ and $4I \approx \pi$.

1. Write a python code to estimate π.

2. Study the accuracy of the approximation as a function of n, the number of samples and deduce the rate of convergence.

3. [Optional] Plot the sample points, red for those under the curve, blue for those above.

Ex. 2: Monte Carlo Integration

Rejection Sampling

Suppose that we want to sample from a multi-modal Gaussian

$$p(x) = \alpha_1 \mathcal{N}(\mu_1, \sigma_1^2) + \alpha_2 \mathcal{N}(\mu_2, \sigma_2^2),$$

but we have no way to accurately sample it because of the two modes.

1. A suitable proposal distribution $q(x)$ would be a simple, unimodal Gaussian, centered between the two modes and with a variance large enough to cover the range of p. Propose and plot a suitable $q(x)$ and superpose it on $p(x)$.

2. By trail and error, find a factor k that is large enough to provide an envelope, i.e. such that $kq(x) \geq p(x)$. Plot again the superposition, but this time with $kq(x)$ and $p(x)$.

3. Perform rejection sampling and plot the accepted sampling points (dots and histograms) for $n = 10^3$ and $n = 10^4$.

Ex. 3: Monte Carlo Integration

Importance Sampling

Suppose that we want to estimate a tail probability, or extreme event probability, of a standard Gaussian, $\mathcal{N}(0,1)$, for $\mathrm{P}(X > 5)$.

- Ordinary MC integration will not be very efficient since almost all the samples will be rejected.
- A better option would be to use an exponential density, truncated at $x = 5$, as the importance function for Importance Sampling

1. Show that ordinary Monte Carlo would result in approximately 3 samples out of 10,000,000 from $\mathcal{N}(0,1)$. to have a value greater than 5. Conclusion?
2. We can use the exponential density truncated at 5 as the importance (proposal) function and use importance sampling to estimate the probability.

(a) Use standard MC to estimate the probability.
(b) Plot the truncated exponential density and the standard Gaussian around the $x = 5$.
(c) Use importance sampling, with the same number of sample points, and compare the result with the theoretical value. Conclusions?

Ex. 4: MC - Rejection Sampling

Prove that rejection sampling draws samples from the desired distribution $p(\mathbf{z})$.

1. Suppose the proposal distribution is $q(\mathbf{z})$. Show that the probability of a sample value $\mathbf{z}$ being accepted is given by $\tilde{p}(\mathbf{z})/kq(\mathbf{z})$ where $\tilde{p}$ is any unnormalized distribution that is proportional to $p(\mathbf{z})$, and the constant k is set to the smallest value that ensures $kq(\mathbf{z}) \geq \tilde{p}(\mathbf{z})$ for all values of $\mathbf{z}$.

2. Note that the probability of drawing a value $\mathbf{z}$ is given by the probability of drawing that value from $q(\mathbf{z})$ times the probability of accepting that value given that it has been drawn. Make use of this, along with the sum and product rules of probability, to write down the normalized form for the distribution over $\mathbf{z}$, and show that it equals $p(\mathbf{z})$.

MARKOV CHAIN

Markov Chains

Principles and Basics

Markov chains are an essential component of Markov chain Monte Carlo (McMC) techniques. Under MCMC, the Markov chain is used to sample from some target distribution. To get a better understanding of what a Markov chain is, and further, how it can be used to sample form a distribution, the following exercises introduce some basic concepts.

- Recall: A Markov chain is defined by three elements:
  - ⇒ A state space x, which is a set of values that the chain is allowed to take.
  - ⇒ A transition operator $p(x^{(t+1)}|x^{(t)})$ that defines the probability of moving from state $x^{(t)}$ to $x^{(t+1)}$.
  - ⇒ An initial condition distribution$\pi^{(0)}$ which defines the probability of being in any one of the possible states at the initial iteration $t = 0$.

- If the transition operator for a Markov chain does not change across transitions, the Markov chain is called time homogenous, and as $t \to \infty$, the chain will reach an equilibrium that is called the chain's stationary distribution, $p(x^{(t+1)}|x^{(t)}) = p(x^{(t)}|x^{(t-1)})$

- The stationary distribution of a Markov chain is important for sampling from probability distributions, a technique that is at the heart of Markov Chain Monte Carlo (McMC) methods.

Ex. 5a: Markov Chains

Continuous

- Finite state-space (time homogenous) Markov chain

  $\Rightarrow$ If the state space of a Markov chain takes on a finite number of distinct values, and it is time homogenous, then the transition operator can be defined by a matrix P, where the entries of P are

$$p_{ij} = p(X^{(t+1)} = j | x^{(t)} = i)$$

  $\Rightarrow$ This means that if the chain is currently in the i-th state, the transition operator assigns the probability of moving to the j-th state by the entries of i-th row of P (i.e. each row of P defines a conditional probability distribution on the state space).

- Consider the problem of predicting the weather in Berkeley, CA. Suppose that

⇒ there are only 3 weather conditions: sunny (s), foggy (f), rainy (r), i.e. a state space that takes on 3 discrete values;

⇒ weather patterns are very stable there, so a Berkeley meteorologist (based on meteorological archives) can easily predict the weather next week based on the weather today with the following transition rules:

→ if it is sunny today, then it is highly likely that it will be sunny next week

$$p(X^{(t+1)} = \mathrm{s} | X^{(t)} = \mathrm{s}) = 0.8,$$

it is very unlikely that it will be raining next week

$$p(X^{(t+1)} = \mathrm{r} | X^{(t)} = \mathrm{s}) = 0.05,$$

and somewhat likely that it will foggy next week

$$p(X^{(t+1)} = \mathrm{f} | X^{(t)} = \mathrm{s}) = 0.15$$

→ if it is foggy today, then it is somewhat likely that it will be sunny next week

$$p(X^{(t+1)} = \mathrm{s} | X^{(t)} = \mathrm{f}) = 0.4,$$

it is slightly more likely that it will be foggy next week

$$p(X^{(t+1)} = \mathrm{f} | X^{(t)} = \mathrm{f}) = 0.5,$$

and fairly unlikely that it will rainy next week

$$p(X^{(t+1)} = \mathrm{r} | X^{(t)} = \mathrm{f}) = 0.1$$

→ if it is rainy today, then it is unlikely that it will be sunny next week

$$p(X^{(t+1)} = \mathrm{s} | X^{(t)} = \mathrm{r}) = 0.1,$$

it is somewhat likely that it will be foggy next week

$$p(X^{(t+1)} = \mathrm{f} | X^{(t)} = \mathrm{r}) = 0.3,$$

and fairly likely that it will be rainy next week

$$p(X^{(t+1)} = \mathrm{r} | X^{(t)} = \mathrm{r}) = 0.6.$$

1. Write the 3×3 transition matrix P, where each row of P corresponds to the weather at iteration t (today), and each column corresponds to the weather at iteration $t + 1$ (next week.)

2. Simulate the evolution of the Markov chain, starting from an initial state of rain, for 6 months (25 week, say).

3. At what point in time does the chain reach a steady equilibrium, and what are the 3 equilibrium probabilities?

4. [Optional] Compute the theoretical steady state by an eigenvector analysis and print the errors.

Ex. 5b: Markov Chains

Continuous

We can use the stationary distribution of a continuous state-space Markov chain in order to sample from a continuous probability distribution: we run a Markov chain for a sufficient amount of time so that it has reached its stationary distribution, then keep the states that the chain visits as samples from that stationary distribution.

In this exercise we define a continuous state-space Markov chain, by supposing:

- The transition operator is a Gaussian distribution with unit variance and a mean that is half the distance between zero and the previous state, and
- the distribution over initial conditions is a Gaussian distribution with zero mean and unit variance.

To ensure that the chain has moved sufficiently far from the initial conditions and that we are sampling

from the chain's stationary distribution, we will choose to throw away the first 50 burn-in states of the chain. We also run multiple chains simultaneously in order to sample the stationary distribution more densely. Here we will choose to run 5 chains simultaneously.

1. Write a code that simulates the 5 chains simultaneously for 1000 iterations.

2. Plot

   (a) a zoom of the first 100 iterations, and mark the burn-in cutoff,
   (b) the complete trace of the 5 chains,
   (c) the histogram of the retained states.

3. What is the stationary distribution? What are its estimated parameters?

4. [Optional] Identifying the chain as an AR(1) process, compute the theoretical variance and compare it with the value obtained from the simulations of the Markov chain.

McMC

Approaches & Methods

- Q: "How does the inference actually work? How do we get these magical samples from the posterior?"

- A: "Well it's easy, MCMC generates samples from the posterior distribution by constructing a reversible Markov-chain that has as its equilibrium distribution the target posterior distribution. Questions?". `https://twiecki.io/blog/2015/11/10/mcmc-sampling/`

  ⇒ Theory is quite clear, but requires deeper understanding of Markov chains and ergodicity.

  ⇒ Practice is somewhat more complex, and needs to be exercised, manipulated, tested, tuned.

- McMC flavors:

  ⇒ Metropolis Hastings is the simplest, and can be viewed as a random walk approach.

⇒ Gibbs Sampling factorizes a complex posterior into the product of simpler, tractable, known posteriors.

⇒ Hamiltonian MC attempts to avoid the "wandering" of the random walk, by introducing dynamics defined by a Hamiltonian system of equations.

Ex. 6: McMC

Metropolis Hastings

[Optional] Go to `https://twiecki.io/blog/2015/11/10/mcmc-sampling/`, follow the explanations and (re)code this very detailed and well-explained MH version of McMC.

Ex. 7: McMC

Metropolis Hastings

This instructive exercise will be in two parts:

1. We will use the Metropolis-Hasting algorithm to compute the posterior distribution of the mean of a Gaussian distribution with known variance, from a sequence of given observations.

2. We will study the influence of the proposal distribution on the convergence of the Markov Chain generated in the first part.

In the first part, we will start with a proposal that is far from the reality, and the likelihood function will also be very approximate. In the second part, we will investigate more closely the behavior of the chain as the proposal distribution changes.

Recall Bayes' Law that gives an expression for the

posterior conditional probability of a parameter θ

$$p(\theta \mid y) = \frac{p(\theta)p(y \mid \theta)}{\int p(\theta')p(y \mid \theta') \, \mathrm{d}\theta'},$$

where y is the observation, $p(\theta)$ is the prior probability, $p(y \mid \theta)$ is the likelihood function and the denominator is a normalization factor representing the total probability of y. Very often, in practical applications, this denominator is intractable (impossible, or too expensive to compute), whereas the likelihood and prior are known. This is an ideal instance for MCMC, since we can simulate the posterior without having to know the normalizing factor.

Consider a simple problem, where we have a sequence of 5 measurements (or samples), $\{y_1, \ldots, y_5\} = \{9.37, 10.18, 9.16, 11.60, 10.33\}$, depending on a parameter θ (the unknown mean) for which we would like to obtain the (posterior) probability distribution, $p(\theta \mid y)$.

For the Metropolis-Hasting algorithm, use the

Metropolis acceptance ratio

$$r = \frac{p\left(\theta^* \mid y\right)}{p\left(\theta^{(t)} \mid y\right)} = \frac{p\left(y \mid \theta^*\right) p(\theta^*)}{p\left(y \mid \theta^{(t)}\right) p(\theta^{(t)})},$$

where θ^* is a candidate value for the chain drawn from the symmetric Gaussian proposal distribution $\mathcal{N}(0, \delta^2)$, the actual value in the chain is denoted $\theta^{(t)}$, the known prior is $\mathcal{N}(\mu, \tau^2)$, and the likelihood is computed assuming that $y_i \sim \mathcal{N}(\theta, \sigma^2)$. The exact expressions for the sample mean and variance can be computed, and are given by

$$\mu_n = \frac{(n/\sigma^2)\bar{y} + (1/\tau^2)\mu}{n/\sigma^2 + 1/\tau^2}$$

and

$$\tau_n^2 = \frac{1}{n/\sigma^2 + 1/\tau^2}.$$

1. Suppose that the proposal distribution has variance $\delta^2 = 2$, and that the prior has parameters $\mu = 5$,

$\tau^2 = 10$. Fix a chain length of 10^4 and an initial value $\theta^{(0)} = 5$. Assume that the likelihood variance is known, with $\sigma^2 = 1$.

(a) Code and simulate the MH algorithm for these values.

(b) Plot the trace (θ as a function of the iteration number, subsampling one in every ten values) and the histogram of the Markov chain (after removing a burn-in period of the first 50 values, say) and compare it with the theoretical law.

(c) Conclusions?

2. We now study how the choice of the parameter δ in the proposal distribution affects the mixing, and hence the convergence of the simulated Markov chain. Consider a sequence of values

$$\delta^2 \in \left\{ \frac{1}{32}, \frac{1}{2}, 2, 32, 64 \right\}.$$

(a) For diagnostic purposes compute the autocorrelation function and record the the lag-1 autocor-

relations. For which value of δ^2 do we have a minimum (optimum)?

(b) Plot and compare the convergence of the 5 Markov chains for the first 500 iterations, one graphic for each value of δ^2. Observations and conclusions?

McMC

Hamiltonian Dynamics - Theory

- Hamiltonian dynamics is one way that physicists describe how objects move throughout a system. Hamiltonian dynamics describe an object's motion in terms of its location $\mathbf{x}$ and momentum $\mathbf{p}$ (equivalent to the object's mass times its velocity) at some time t.

- For each location the object takes, there is an associated potential energy $U(\mathbf{x})$, and for each momentum there is an associated kinetic energy $K(\mathbf{p})$. The total energy of the system is constant and known as the Hamiltonian $H(\mathbf{x}, \mathbf{p})$ defined simply as the sum of the potential and kinetic energies,

$$H(\mathbf{x}, \mathbf{p}) = U(\mathbf{x}) + K(\mathbf{p}).$$

- Hamiltonian dynamics describe how kinetic energy is converted to potential energy (and vice versa) as

an object moves throughout a system in time. This description is implemented quantitatively via a set of differential equations known as the Hamiltonian equations,

$$\frac{\partial x_i}{\partial t} = \frac{\partial H}{\partial p_i} = \frac{\partial K(\mathbf{p})}{\partial p_i},$$
$$\frac{\partial p_i}{\partial t} = -\frac{\partial H}{\partial x_i} = -\frac{\partial U(\mathbf{x})}{\partial x_i}.$$

- Therefore, if we have expressions for $\partial U(\mathbf{x})/\partial x_i$ and $\partial K(\mathbf{p})/\partial p_i$ and a set of initial conditions (i.e. an initial position $\mathbf{x}_0$ and initial momentum $\mathbf{p}_0$ at time t_0), it is possible to predict the location and momentum of an object at any point in time $t = t_0 + T$ by simulating these dynamics for a duration T.

McMC

Hamiltonian Dynamics - Numerics

- There are a number of numerical methods for discretizing the dynamics in time, including Euler's method and the Leapfrog Method

- The Leapfrog method updates the momentum and position variables sequentially, starting by simulating the momentum dynamics over a small interval of time $\delta/2$, then simulating the position dynamics over a slightly longer interval in time δ, then completing the momentum simulation over another small interval of time $\delta/2$ so that $\mathbf{x}$ and $\mathbf{p}$ now exist at the same point in time.

  $\Rightarrow$ a half step in time to update the momentum variable
  $\Rightarrow$ a full step in time to update the position variable
  $\Rightarrow$ the remaining half step in time to finish updating

the momentum variable

$$p_i\left(t+\frac{\delta}{2}\right) = p_i(t) - \frac{\delta}{2}\frac{\partial U}{\partial x_i}(t)$$

$$x_i(t+\delta) = x_i(t) + \delta\frac{\partial K}{\partial p_i}\left(t+\frac{\delta}{2}\right)$$

$$p_i(t+\delta) = p_i\left(t+\frac{\delta}{2}\right) - \frac{\delta}{2}\frac{\partial U}{\partial x_i}(t+\delta)$$

$\Rightarrow$ this scheme is symplectic (area-preserving)... unlike Euler, Runge-Kutta, etc.

Ex. 8: McMC

HMC - Harmonic Oscillator

The objective here is to demonstrates the leapfrog integration method for Hamiltonian dynamics, showing how the harmonic oscillator evolves in time, while conserving total energy in phase space. The code for the simulation of the dynamics can be utilized, as is, for Hamiltonian Monte Carlo—see below.

- The obtained results should clearly demonstrate the physics:

  $\Rightarrow$ the harmonic oscillator exhibits periodic motion,
  $\Rightarrow$ energy oscillates between kinetic and potential forms while total energy remains constant,
  $\Rightarrow$ and the phase space trajectory traces out an ellipse characteristic of conservative Hamiltonian systems.

- Suppose a ball of mass $m = 1$ is attached to a horizontal spring (no gravity). Then the spring

exerts a force on the ball

$$F = -kx,$$

where k is the spring constant, which we suppose equal to one.

- The potential energy is then

$$U(x) = \int F \, \mathrm{d}x = \int -x \, \mathrm{d}x = -\frac{x^2}{2}$$

and the kinetic energy

$$K(v) = \frac{1}{2}mv^2 = \frac{v^2}{2} = \frac{p^2}{2} = K(p).$$

Their partial derivatives are

$$\frac{\partial U(x)}{\partial x} = x, \quad \frac{\partial K(p)}{\partial p} = p.$$

1. Write down the Hamiltonian and the 3 steps of the leapfrog method for the Hamiltonian system.

2. Simulate the dynamics, with $\delta = 0.1$ for 70 time steps. Use the initial conditions: position $x(0) = -4$, momentum $p(0) = 1$.

3. Plot:

   (a) position as a function of time,
   (b) U, K and H as a function of time,
   (c) the phase plot, in the $x - p$ plane.

HMC

Theory and algorithm

- This is a foundational example that demonstrates how HMC combines the best aspects of Hamiltonian dynamics simulation with Bayesian sampling, making it especially powerful for high-dimensional posterior distributions in modern statistical computing.

- Recall:

  $\Rightarrow$ The random-walk behavior of many Markov Chain Monte Carlo (McMC) algorithms makes Markov chain convergence to a target stationary distribution $p(x)$ inefficient, resulting in slow mixing.

  $\Rightarrow$ Hamiltonian/Hybrid Monte Carlo (HMC), is a McMC method that adopts physical system dynamics rather than a probability distribution to propose future states in the Markov chain.

⇒ This allows the Markov chain to explore the target distribution much more efficiently, resulting in faster convergence.

⇒ The main idea behind Hamiltonian/Hybrid Monte Carlo is to develop a Hamiltonian function $H(\mathbf{x}, \mathbf{p})$ such that the resulting Hamiltonian dynamics allow us to efficiently explore some target distribution $p(\mathbf{x})$.

- How can we choose such a Hamiltonian function? It turns out it is pretty simple to relate a $H(\mathbf{x}, \mathbf{p})$ to $p(\mathbf{x})$ using a basic concept adopted from statistical mechanics known as the canonical distribution.

  ⇒ For any energy function $E(\theta)$ over a set of variables θ, we can define the corresponding canonical distribution as

$$p(\theta) = \frac{1}{Z} e^{-E(\theta)}$$

  where we simply take the exponential of the negative of the energy function.

⇒ The variable Z is a normalizing constant called the partition function that scales the canonical distribution such that is sums to one, creating a valid probability distribution.

⇒ Now, as we saw above, the energy function for Hamiltonian dynamics is a combination of potential and kinetic energies

$$E(\theta) = H(\mathbf{x}, \mathbf{p}) = U(\mathbf{x}) + K(\mathbf{p})$$

⇒ Therefore the canonical distribution for the Hamiltonian dynamics energy function is

$$\begin{aligned} p(\mathbf{x}, \mathbf{p}) &\propto e^{-H(\mathbf{x},\mathbf{p})} \\ &= e^{-[U(\mathbf{x})+K(\mathbf{p})]} \\ &= e^{-U(\mathbf{x})} e^{-K(\mathbf{p})} \\ &\propto p(\mathbf{x})p(\mathbf{p}) \end{aligned}$$

⇒ Here we see that joint (canonical) distribution for $\mathbf{x}$ and $\mathbf{p}$ factorizes. This means that the two variables are independent, and the canoncial dis-

tribution $p(\mathbf{x})$ is independent of the analogous distribution for the momentum. Therefore, we can use Hamiltonian dynamics to sample from the joint canonical distribution over $\mathbf{p}$ and $\mathbf{x}$ and simply ignore the momentum contributions. Note that this is an example of introducing auxiliary variables to facilitate the Markov chain path. Introducing the auxiliary variable $\mathbf{p}$ allows us to use Hamiltonian dynamics, which are unavailable without them.

$\Rightarrow$ Because the canonical distribution for $\mathbf{x}$ is independent of the canonical distribution for $\mathbf{p}$, we can choose any distribution from which to sample the momentum variables. A common choice is to use a zero-mean, normal distribution with unit variance, that is

$$p(\mathbf{p}) \propto \frac{\mathbf{p}^\top \mathbf{p}}{2}.$$

Note that this is equivalent to having a quadratic

potential energy term in the Hamiltonian

$$K(\mathbf{p}) = \frac{\mathbf{p}^\top \mathbf{p}}{2},$$

which is the exact quadratic kinetic energy function (albeit in 1D) used in the harmonic oscillator example above, and is simple to differentiate.

$\Rightarrow$ Now that we have defined a kinetic energy function, all we have to do is find a potential energy function $U(\mathbf{x})$ that when negated and run through the exponential function, gives the target distribution $p(\mathbf{x})$ (or an unscaled version of it). In other words, we can simply define the potential energy function as

$$U(\mathbf{x}) = -\log p(\mathbf{x}),$$

and if we can calculate its partial derivative with respect to x, we will have all the ingredients for simulating Hamiltonian dynamics that can be used in an McMC technique.

- HMC: we use Hamiltonian dynamics as a proposal function for a Markov chain in order to explore the target (canonical) density $p(\mathbf{x})$ defined by $U(\mathbf{x})$ more efficiently than using a proposal probability distribution.

  $\Rightarrow$ Starting at an initial state$[\mathbf{x}_0, \mathbf{p}_0]$, we simulate Hamiltonian dynamics for a short time using the Leapfrog method.

  $\Rightarrow$ We then use the state of the position and momentum variables at the end of the simulation as our proposed state variables $\mathbf{x}^*$ and $\mathbf{p}^*$.

  $\Rightarrow$ The proposed state is accepted using an update rule analogous to the Metropolis acceptance criterion.

- For a given set of initial conditions, Hamiltonian dynamics will follow contours of constant energy in phase space (analogous to the circle traced out in phase space in the example above). Therefore we must randomly perturb the dynamics so as to explore all of $p(\mathbf{x})$. This is done by simply drawing a random momentum from the corresponding canon-

ical distribution $p(\mathbf{p})$ before running the dynamics prior to each sampling iteration t.

- Combining these steps:

  $\Rightarrow$ sampling random momentum,
  $\Rightarrow$ followed by Hamiltonian dynamics
  $\Rightarrow$ and Metropolis acceptance criterion,

- defines the HMC algorithm for drawing M samples from a target distribution.

HMC

Algorithm

1. set $t = 0$

2. generate an initial position state $\mathbf{x}^{(0)} \sim \pi^{(0)}$

3. repeat until $t = M$

   (a) set $t = t + 1$
   (b) sample a new initial momentum variable from the momentum canonical distribution $\mathbf{p}_0 \sim p(\mathbf{p})$
   (c) set $\mathbf{x}_0 = \mathbf{x}^{(t-1)}$.
   (d) run Leapfrog algorithm starting at $[\mathbf{x}_0, \mathbf{p}_0]$ for L steps and step-size δ to obtain proposed states $\mathbf{x}^*$ and $\mathbf{p}^*$
   (e) calculate the Metropolis acceptance probability:

$$\begin{aligned}\alpha &= \min(1, \exp(-U(\mathbf{x}^*) + U(\mathbf{x}_0) - K(\mathbf{p}^*) + K(\mathbf{p}_0))) \\ &= \min\left(1, \exp\left(H(\mathbf{x}_0) - H(\mathbf{x}^*)\right)\right)\end{aligned}$$

(f) draw a random number u from Unif$(0, 1)$
   i. if $u \leq \alpha$ accept the proposed state position $\mathbf{x}^*$ and set the next state in the Markov chain $\mathbf{x}^{(t)} = \mathbf{x}^*$
   ii. else set $\mathbf{x}^{(t)} = \mathbf{x}^{(t-1)}$

Ex. 9: McMC

HMC - Sampling from bivariate Gaussian

The target distribution $p(\mathbf{x})$ for this sampling exercise is a bivariate Gaussian with the following parameterization: $p(\mathbf{x}) = \mathcal{N}(\mu, \mathbf{\Sigma})$ with mean $\mu = [\mu_1, \mu_2] = [0, 0]$ and covariance

$$\mathbf{\Sigma} = \begin{bmatrix} 1 & \rho_{12} \\ \rho_{21} & 1 \end{bmatrix} = \begin{bmatrix} 1 & 0.8 \\ 0.8 & 1 \end{bmatrix}.$$

In order to sample from $p(\mathbf{x})$ (assuming that we are using a quadratic energy function), we need to determine the expressions for $U(\mathbf{x})$ and $\partial U(\mathbf{x})/\partial x_i$. Recall that the target potential energy function can be defined from the canonical form as $U(\mathbf{x}) = -\log(p(\mathbf{x}))$. So, taking the negative log of the Gaussian distribution above, we define the potential energy function

$$E(\mathbf{x}) = -\log\left(e^{-\frac{\mathbf{x}^\mathbf{T}\mathbf{\Sigma}^{-1}\mathbf{x}}{2}}\right) - \log Z,$$

where Z is the normalizing constant for a Gaussian distribution and can be ignored because it will cancel. The potential energy function is then simply,

$$U(\mathbf{x}) = \frac{\mathbf{x^T \Sigma^{-1} x}}{2}$$

with partial derivatives

$$\frac{\partial U(\mathbf{x})}{\partial x_i} = x_i.$$

We are now in possession of all the ingredients for implementing the HMC algorithm.

- The algorithm samples from a bivariate normal distribution with correlation coefficient 0.8. The HMC method is particularly effective for this type of problem because it can make large moves while maintaining high acceptance rates, avoiding the random walk behavior of simpler McMC methods.

Ex 10: FWI using HMC

ADVANCED

- Fichtner's HMC lab paper in *GJI* (2023), 235.

  $\Rightarrow$ use HMCLab to reproduce the results

Ex. 11: FWI using VI

ADVANCED

- Zhang, Curtis review in *Advances in Geophysics*, 62 (2021).

  $\Rightarrow$ use VIP package to reproduce the results

  $\Rightarrow$ compare with HMC