Hamiltonian Monte Carlo

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November 9, 2023

Adapted from Radford Neal's MCMC Using Hamltonian Dynamics in Handbook of Markov Chain Monte Carlo (2011).

Hamiltonian system

Considering a body in a frictionless 1-dimensional environment with

- mass m,
- location θ, and
- momentum $\omega = mv$ where v is velocity.

The mass has

- potential energy $U(\theta)$, proportional to its height, and
- kinetic energy $K(\omega) = \frac{1}{2}mv^2 = \frac{1\omega^2}{2m}$.

Hamilton's equations

Extending this to d dimensions, we have

- position vector θ and
- momentum vector ω.

The Hamiltonian $H(\theta, \omega)$ describes the time evolution of the system through

$$\begin{aligned} \frac{d\theta_i}{dt} &= \frac{\partial H}{\partial \omega_i} \\ \frac{d\omega_i}{dt} &= -\frac{\partial H}{\partial \theta_i} \end{aligned}$$

for $i = 1, \ldots, d$.

Potential and kinetic energy

For Hamiltonian Monte Carlo, we usually use Hamiltonian functions that can be written as follows:

$$H(\theta, \omega) = U(\theta) + K(\omega)$$

where

- $U(\theta)$ is called the potential energy and will be defined to be minus the log probability density of the distribution for θ (plus any constant that is convenient) and
- $K(\omega)$ is called the kinetic energy and is usually defined as

  $$K(\omega) = \omega^\top M^{-1} \omega / 2$$

  where M is a symmetric, positive-definite "mass matrix", which is typically diagonal, and is often a scalar multiple of the identity matrix. This form for $K(\omega)$ corresponds to minus the log probability density (plus a constant) of the zero-mean Gaussian distribution with covariance matrix M.

The resulting Hamilton's equations are

$$\frac{d\theta_i}{dt} = [M^{-1}\omega]_i, \qquad \frac{d\omega_i}{dt} = -\frac{\partial U}{\partial \theta_i}.$$

One-dimensional example

Suppose

$$H(\theta,\omega) = U(\theta) + K(\omega), \quad U(\theta) = \theta^2/2, \quad K(\omega) = \omega^2/2$$

The dynamics resulting from this Hamiltonian are

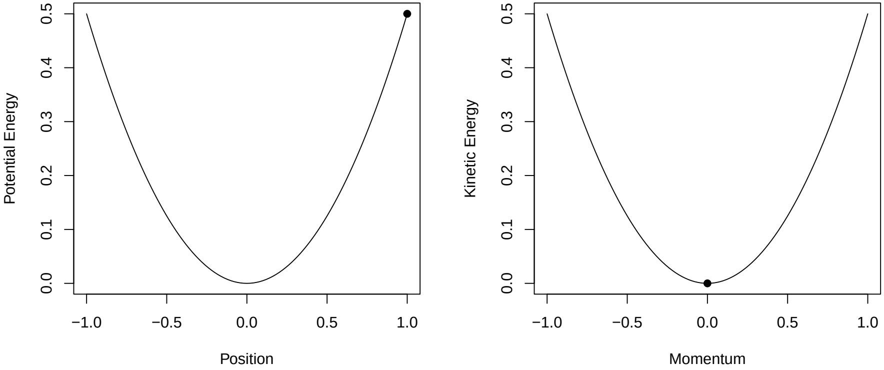
$$\frac{d\theta}{dt} = \omega, \quad \frac{d\omega}{dt} = -\theta.$$

Solutions are of the form

$$\theta(t) = r\, cos(a+t), \quad \omega(t) = -r\, sin(a+t)$$

for some constants r and a that depend on initial conditions.

One-dimensional example simulation

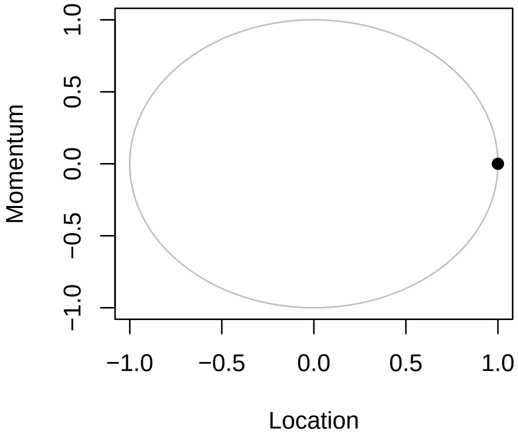


Conservation of the Hamiltonian

This simple model clearly conserves the Hamiltonian:

$$\begin{aligned}
H(\theta,\omega) &= U(\theta) + K(\omega) \\
&= \frac{\theta^2}{2} + \frac{\omega^2}{2} \\
&= \frac{[r\, cos(a+t)]^2}{2} + \frac{[-r\, sin(a+t)]^2}{2} \\
&= \frac{r^2}{2}\left[cos^2(a+t) + sin^2(a+t)\right] \\
&= r^2/2
\end{aligned}$$

Conservation of the Hamiltonian



Conservation of the Hamiltonian

The dynamics conserve the Hamiltonian since

$$\begin{aligned} \frac{dH}{dt} &= \sum_{i=1}^{d} \left[\frac{d\theta_i}{dt}\frac{\partial H}{\partial \theta_i} + \frac{d\omega_i}{dt}\frac{\partial H}{\partial \omega_i} \right] \\ &= \sum_{i=1}^{d} \left[\frac{\partial H}{\partial \omega_i}\frac{\partial H}{\partial \theta_i} - \frac{\partial H}{\partial \theta_i}\frac{\partial H}{\partial \omega_i} \right] \end{aligned}$$

If H is conserved, then the acceptance probability based on Hamiltonian dynamics is 1. Simulating most Hamiltonian systems, we can only make H approximately conserved.

Reversibility

Hamiltonian dynamics is reversible, i.e. the mapping T_s from the state at time t, $(\theta(t), \omega(t))$, to the state at time $t+s$, $(\theta(t+s), p(t+s))$, is one-to-one, and hence as an inverse, T_{-s}. Under our usual assumptions for HMC, the inverse mapping can be obtained by negating ω, applying T_s, and then negating ω again. The reversibility of Hamiltonian dynamics is important for showing convergence of HMC.

Volume preservation

If we apply the mapping T_s to points in some region R in (θ, ω) space with volume V, the image of R under T_s will also have volume V. This feature simplifies calculation of the acceptance probability for Metropolis updates.

Euler's method

For simplicity, assume

$$H(\theta,\omega) = U(\theta) + K(\omega), \qquad K(\omega) = \sum_{i=1}^{d} \frac{\omega_i^2}{2m_i}.$$

One way to simulate Hamiltonian dynamics is to discretize time into increments of e, i.e.

$$\begin{array}{lll} \omega_i(t+e) & = \omega_i(t) + e\frac{d\omega_i}{dt}(t) & = \omega_i(t) - e\frac{\partial U}{\partial \theta_i}(\theta(t)) \\ \theta_i(t+e) & = \theta_i(t) + e\frac{d\theta_i}{dt}(t) & = \theta_i(t) + e\frac{\omega_i(t)}{m_i} \end{array}$$

Leapfrog method

An improved approach is the leapfrog method which has the following updates:

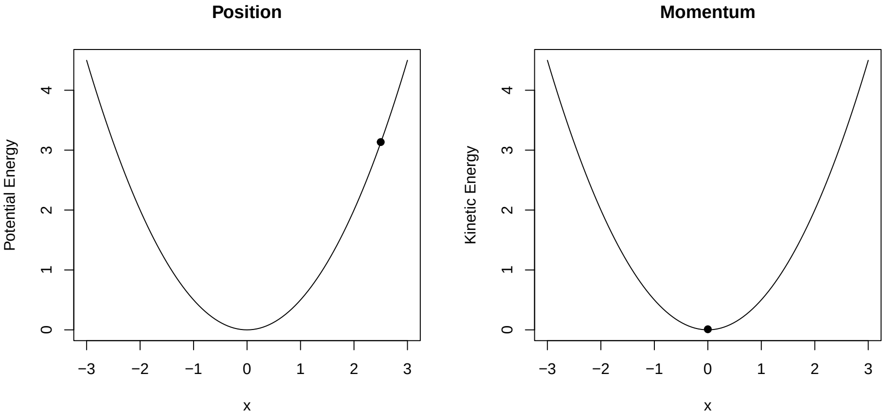
$$\begin{aligned} \omega_i(t+e/2) &= \omega_i(t) - (e/2)\frac{\partial U}{\partial \theta_i}(\theta(t)) \\ \theta_i(t+e) &= \theta_i(t) + e\frac{\omega_i(t+e/2)}{m_i} \\ \omega_i(t+e) &= \omega_i(t+e/2) - (e/2)\frac{\partial U}{\partial \theta_i}(\theta(t+e)) \end{aligned}$$

The leapfrog method is reversible and preserves volume exactly.

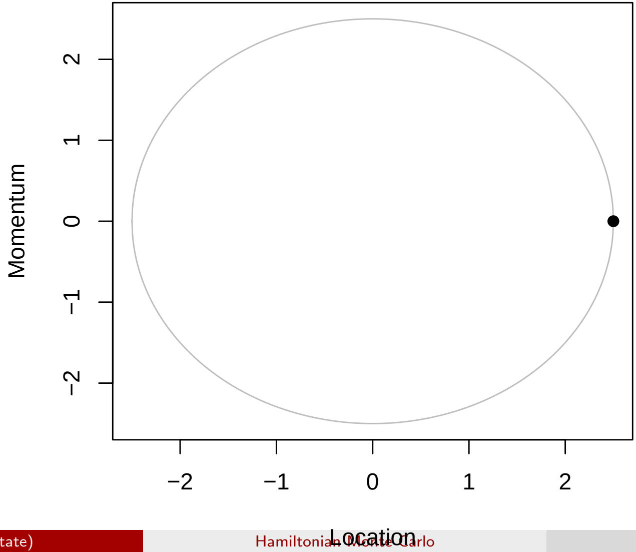
Leap-frog simulator

```
leap_frog = function(U, grad_U, e, L, theta, omega) {
  omega = omega - e/2 * grad_U(theta)

    for (l in 1:L) {
      theta = theta + e * omega
      if (l<L) omega = omega - e * grad_U(theta)
    }
    omega = omega - e/2 * grad_U(theta)
  return(list(theta=theta,omega=omega))
}
```

Leap-frog simulator



Conservation of the Hamiltonian



Probability distributions

The Hamiltonian is an energy function for the joint state of “position”, θ, and “momentum”, ω, and so defines a joint distribution for them, via

$$p(\theta, \omega) = \frac{1}{Z} \exp\left(-H(\theta, \omega)\right)$$

where Z is the normalizing constant.
If $H(\theta, \omega) = U(\theta) + K(\omega)$, the joint density is

$$p(\theta, \omega) = \frac{1}{Z} \exp\left(-U(\theta)\right) \exp\left(-K(\omega)\right).$$

If we are interested in a posterior distribution, we set

$$U(\theta) = -\log\left[p(y|\theta)p(\theta)\right].$$

Hamiltonian Monte Carlo algorithm

Set tuning parameters

- L: the number of steps
- e: stepsize
- $D = \{d_i\}$: covariance matrix for ω

Let $\theta^{(i)}$ be the current value of the parameter θ. The leap-frog Hamiltonian Monte Carlo algorithm is

1. Sample $\omega \sim N_d(0, D)$.
2. Simulate Hamiltonian dynamics on location $\theta^{(i)}$ and momentum ω via the leapfrog method (or any reversible method that preserves volume) for L steps with stepsize e. Call these updated values θ^* and $-\omega^*$.
3. Set $\theta^{(i+1)} = \theta^*$ with probability $\min\{1, \rho(\theta^{(i)}, \theta^*)\}$ where

$$\rho(\theta^{(i)}, \theta^*) = \frac{p(\theta^*|y)}{p(\theta^{(i)}|y)} \frac{p(\omega^*)}{p(\omega^{(i)})} = \frac{p(y|\theta^*)p(\theta^*)}{p(y|\theta^{(i)})p(\theta^{(i)})} \frac{N_d(\omega^*; 0, D)}{N_d(\omega^{(i)}; 0, D)}$$

   otherwise set $\theta^{(i+1)} = \theta^{(i)}$.

Reversibility

Reversibility for the leapfrog means that

- if you simulate from (θ, ω) to (θ^*, ω^*) for some step size e and number of steps L then
- if you simulate from $(\theta^*, -\omega^*)$ for the same e and L, you will end up at $(\theta, -\omega)$.

If we use q to denote our simulation “density”, then reversibility means

$$q(\theta^*, \omega^* | \theta, \omega) = q(\theta, -\omega | \theta^*, -\omega^*)$$

and thus in the Metropolis-Hastings calculation, the proposal is symmetric. In order to ensure reversibility of our proposal, we need to negate momentum after we complete the leap-frog simulation. So long as $q(\omega) = q(-\omega)$, which is true for a multivariate normal centered at 0, this will not affect our acceptance probability.

Conservation of Hamiltonian results in perfect acceptance

The Hamiltonian is conserved if $H(\theta, \omega) = H(\theta^*, \omega^*)$ which implies

$$\begin{aligned} p(\theta^*|y)p(\omega^*) &= \exp\left(-H(\theta^*, \omega^*)\right) \\ &= \exp\left(-H(\theta, \omega)\right) \\ &= p(\theta|y)p(\omega) \end{aligned}$$

and thus the Metropolis-Hastings acceptance probability is

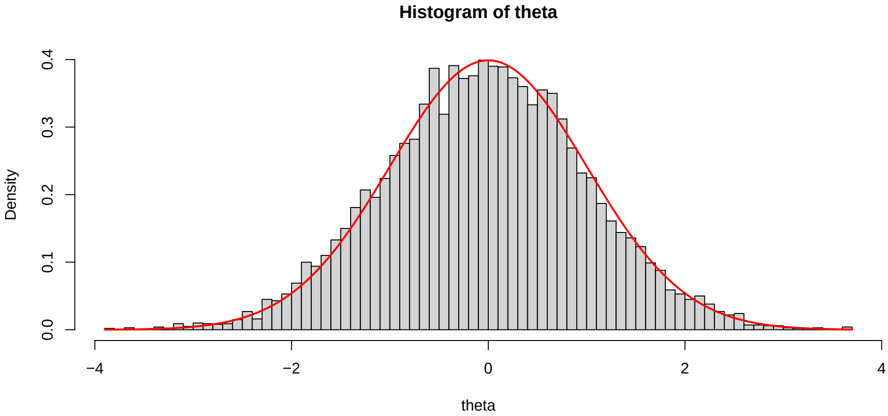
$$\rho(\theta^{(i)}, \theta^*) = \frac{p(\theta^*|y)p(\omega^*)}{p(\theta^{(i)}|y)p(\omega^{(i)})} = 1.$$

This will only be the case if the simulation is perfect! But we have discretization error. The acceptance probability accounts for this error.

```
HMC_neal = function(U, grad_U, e, L, current_theta) {
  theta = current_theta
  omega = rnorm(length(theta),0,1)
  current_omega = omega

  omega = omega - e * grad_U(theta) / 2

  for (i in 1:L) {
    theta = theta + e * omega
    if (i!=L) omega = omega - e * grad_U(theta)
  }
  omega = omega - e * grad_U(theta) / 2

  omega = -omega

  current_U  = U(current_theta)
  current_K  = sum(current_omega^2)/2
  proposed_U = U(theta)
  proposed_K = sum(omega^2)/2

  # cat(paste(e,L,i,theta,omega,"\n"))

  if (runif(1) < exp(current_U-proposed_U+current_K-proposed_K))
  {
    return(theta)
  }
  else {
    return(current_theta)
  }
}
```

```
HMC = function(n_reps, log_density, grad_log_density, tuning, initial) {
  theta = rep(0, n_reps)
  theta[1] = initial$theta

  for (i in 2:n_reps) theta[i] = HMC_neal(U = function(x) -log_density(x),
                                          grad_U = function(x) -grad_log_density(x),
                                          e = tuning$e,
                                          L = tuning$L,
                                          theta[i-1])
  theta
}
```

```
theta = HMC(1e4, function(x) -x^2/2, function(x) -x, list(e=1,L=1), list(theta=0))
hist(theta, freq=F, 100)
curve(dnorm, add=TRUE, col='red', lwd=2)
```



Tuning parameters

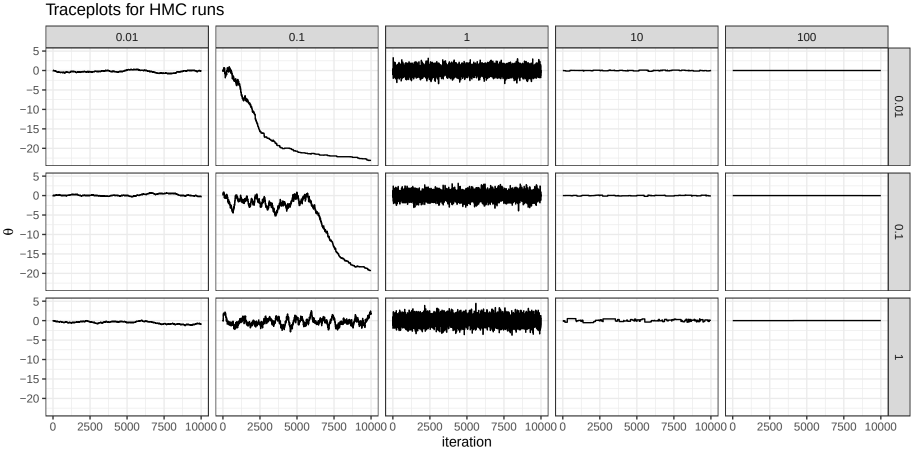
There are three tuning parameters:

- e: step size
- L: number of steps
- D: covariance matrix for momentum

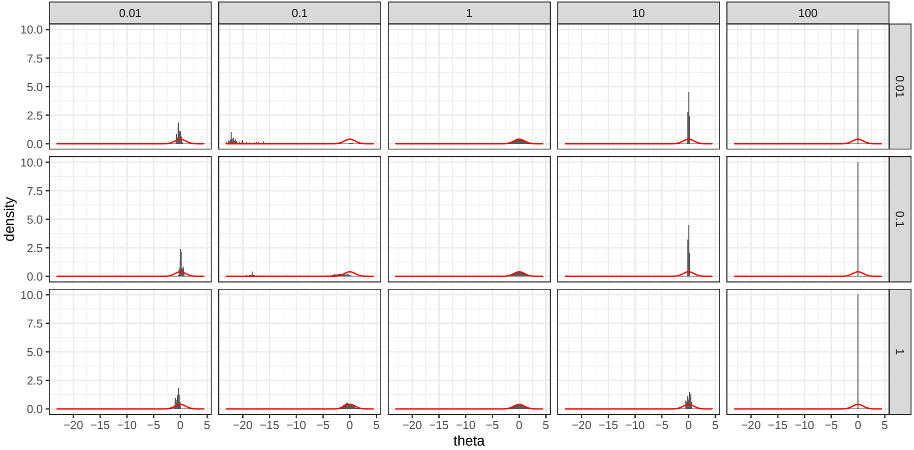
Let $\Sigma = V(\theta|y)$, then an optimal normal distribution for ω is $N(0, \Sigma^{-1})$. Typically, we do not know Σ, but we can estimate it using posterior samples. We can update this estimate throughout burn-in (or warm-up).

Effect of e and L

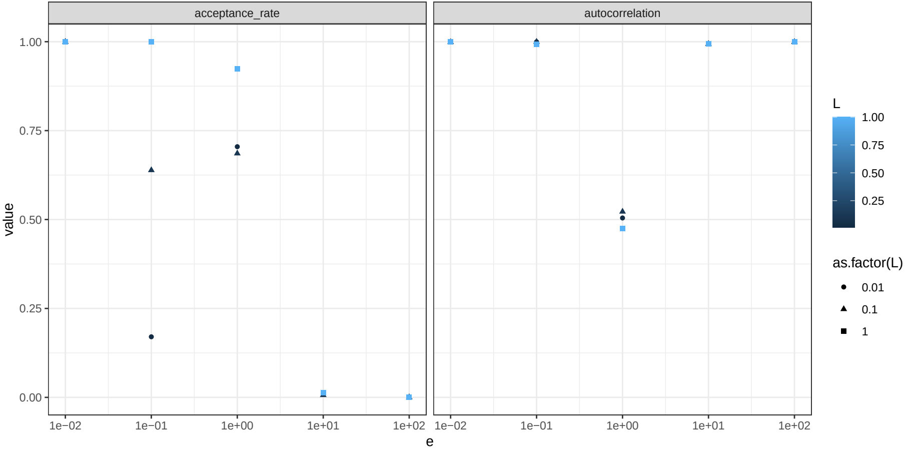
```
n_reps = 1e4
d = expand.grid(e=10^c(-2:2), L=10^c(-2:0))
r = ddply(d, .(e,L), function(xx) {
  data.frame(
    iteration = 1:n_reps,
    theta = HMC(n_reps, function(x) -x^2/2, function(x) -x, list(e=xx$e,L=xx$L), list(theta=0)))
})
```


Traceplots for HMC runs
0.01
0.1
1
10
100
0.01
0.1
1
5
0
−5
−10
−15
−20
θ
0
2500
5000
7500
10000
iteration

```
## Warning:  The dot-dot notation (`..density..`) was deprecated in ggplot2 3.4.0.
## i Please use `after_stat(density)` instead.
## This warning is displayed once every 8 hours.
## Call `lifecycle::last_lifecycle_warnings()` to see where this warning was generated.
```



```
## Warning:  Removed 1 rows containing missing values (‘geom_point()‘).
```



Random-walk vs HMC

https://www.youtube.com/watch?v=Vv3f0QNWvWQ

Summary

Hamiltonian Monte Carlo (HMC) is a Metropolis-Hastings method using parameter augmentation and a sophisticated proposal distribution based on Hamiltonian dynamics such that

- the acceptance probability can be kept near 1
- while still efficiently exploring the posterior.

HMC still requires us to set tuning parameters

- e: step size
- L: number of steps
- D: covariance matrix for momentum

and can only be run in models with continuous parameters in $\mathbb{R}^d$ (or transformed to $\mathbb{R}^d$).