Hamiltonian Monte Carlo

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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, let

- m be its mass,
- q be its position, and
- p be its momentum.

The mass has

- potential energy $U(q)$ (which is proportional to its height) and
- kinetic energy $K(p) = p^2/(2m)$.

Hamilton's equations

Extending this to d dimensions, we have

- position vector q and
- momentum vector p.

The Hamiltonian $H(q, p)$ describes the time evolution of the system through

$$\begin{aligned} \frac{dq_i}{dt} &= \frac{\partial H}{\partial p_i} \\ \frac{dp_i}{dt} &= -\frac{\partial H}{\partial q_i} \end{aligned}$$

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

Potential and kinetic energy

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

$$H(q, p) = U(q) + K(p)$$

where

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

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

  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 $K(p)$ 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

$$\frac{dq_i}{dt} = [M^{-1}p]_i, \qquad \frac{dp_i}{dt} = -\frac{\partial U}{\partial q_i}.$$

One-dimensional example

Suppose

$$H(q,p) = U(q) + K(p), \quad U(q) = q^2/2, \quad K(p) = p^2/2$$

The dynamics resulting from this Hamiltonian are

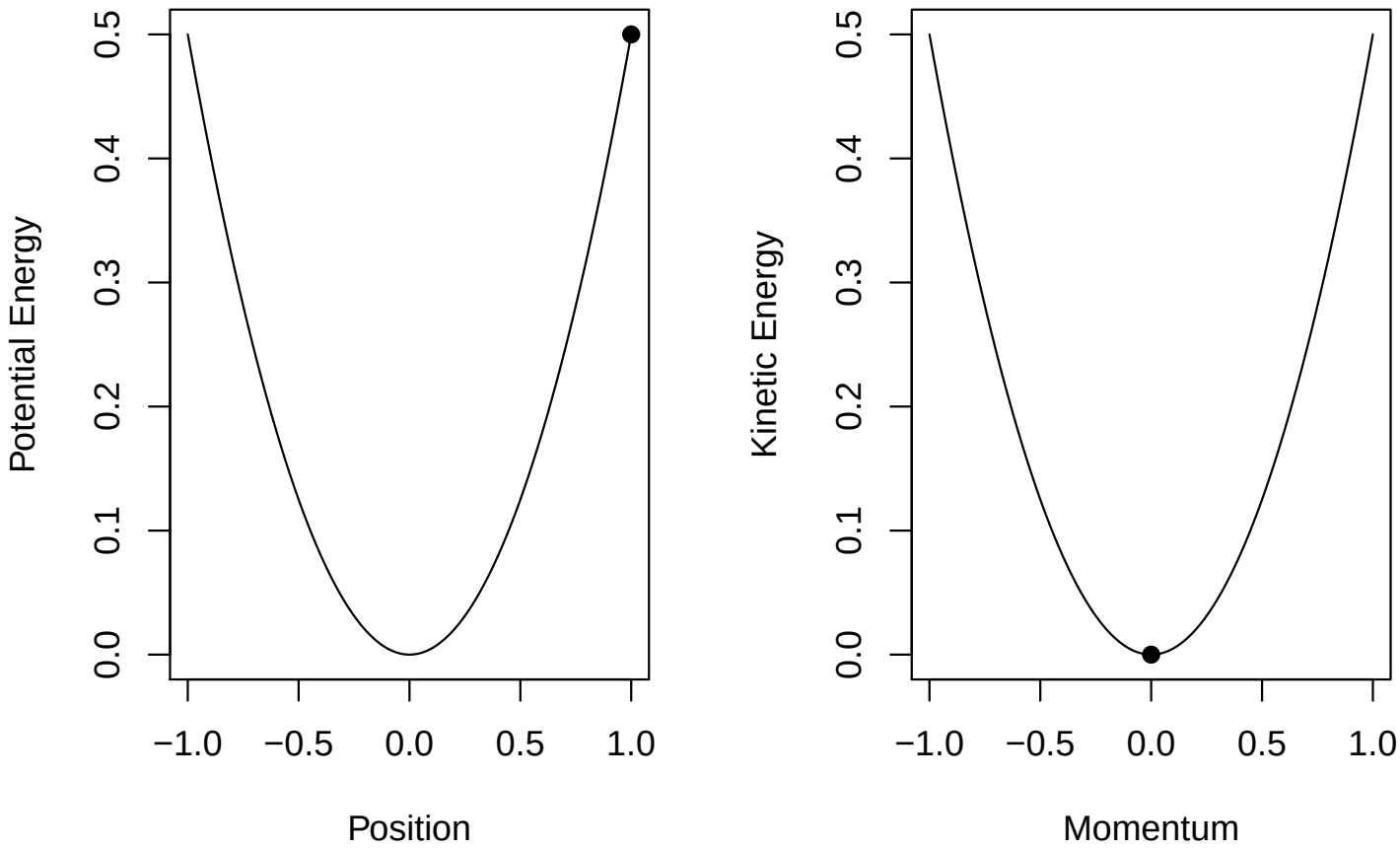
$$\frac{dq}{dt} = p, \quad \frac{dp}{dt} = -q.$$

Solutions of the form

$$q(t) = r\,cos(a+t), \quad p(t) = -r\,sin(a+t)$$

for some constants r and a.

One-dimensional example simulation



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

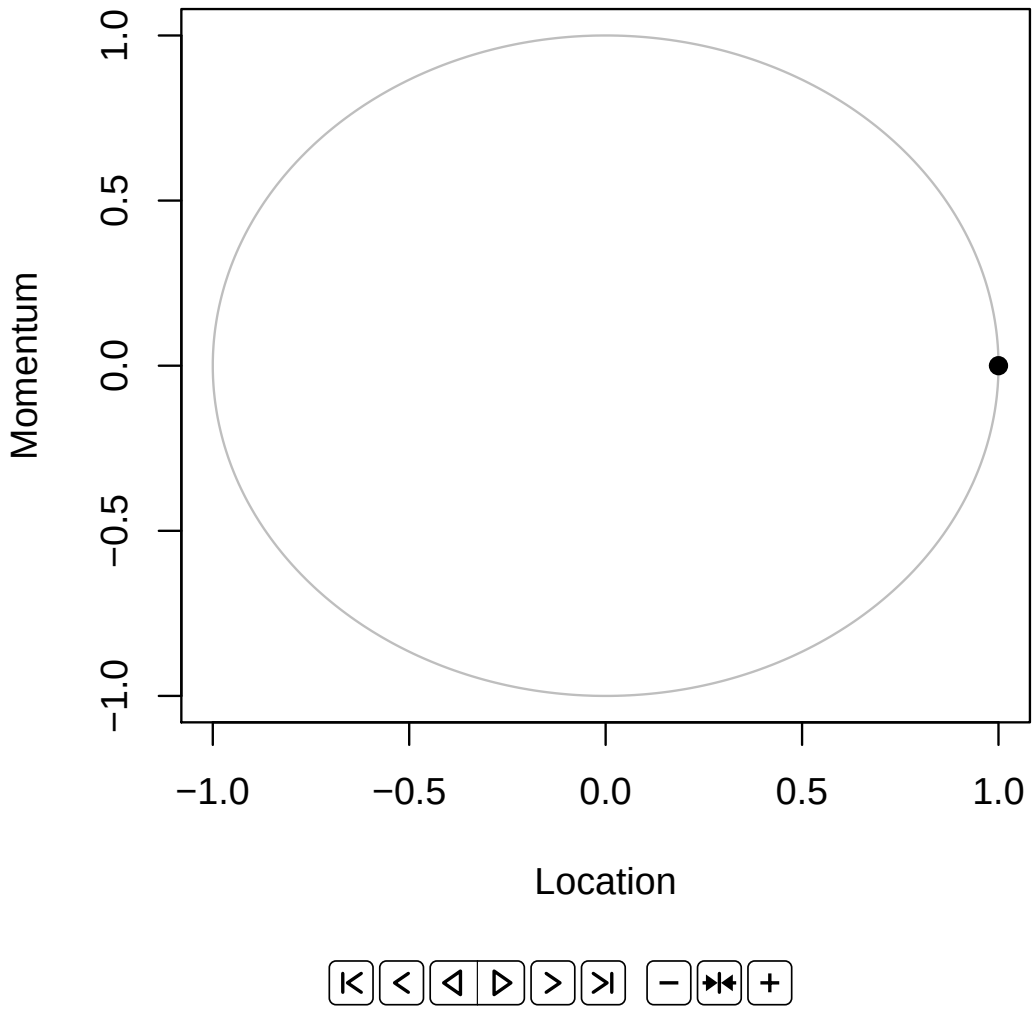
Conservation of the Hamiltonian

The dynamics conserve the Hamiltonian since

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

If h is conserved, then the acceptance probability based on Hamiltonian dynamics is 1. In practice, we can oly make H approximately invariant.

Conservation of the Hamiltonian



Volume preservation

If we apply the mapping T_s to point in some region R of (q, p) 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

$$H(q,p) = U(q) + K(p), \qquad K(p) = \sum_{i=1}^{d} \frac{p_i^2}{2m_i}.$$

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

$$\begin{aligned} p_i(t+e) &= p_i(t) + e\frac{dp_i}{dt}(t) &&= p_i(t) - e\frac{\partial U}{\partial q_i}(q(t)) \\ q_i(t+e) &= q_i(t) + e\frac{dq_i}{dt}(t) &&= q_i(t) + e\frac{p_i(t)}{m_i} \end{aligned}$$

Leapfrog method

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

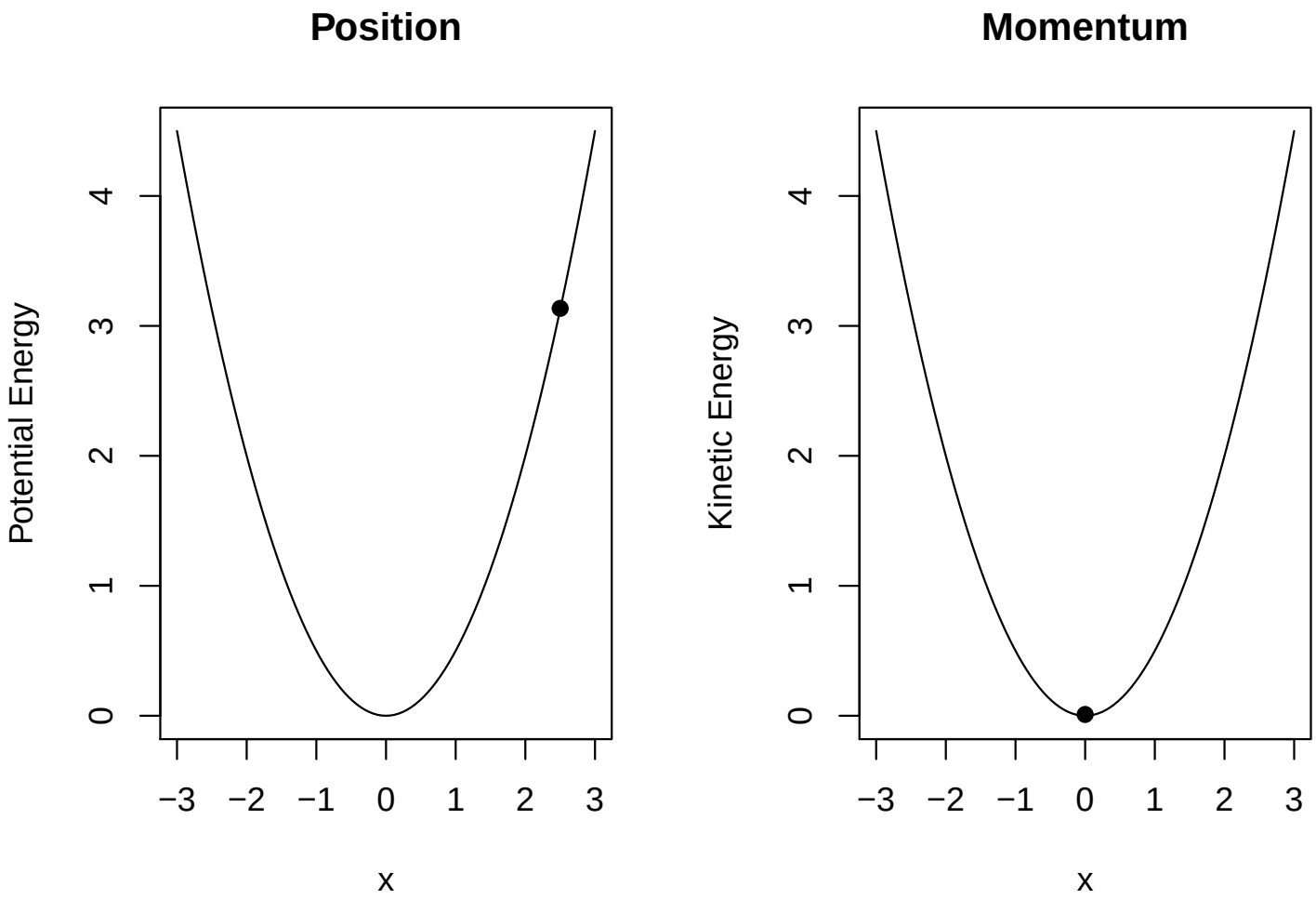
$$\begin{aligned} p_i(t + e/2) &= p_i(t) - (e/2)\frac{\partial U}{\partial q_i}(q(t)) \\ q_i(t + e) &= q_i(t) + e\frac{p_i(t+e/2)}{m_i} \\ p_i(t + e) &= p_i(t + e/2) - (e/2)\frac{\partial U}{\partial q_i}(q(t + e)) \end{aligned}$$

The leapfrog method is reversible and preserves volume exactly.

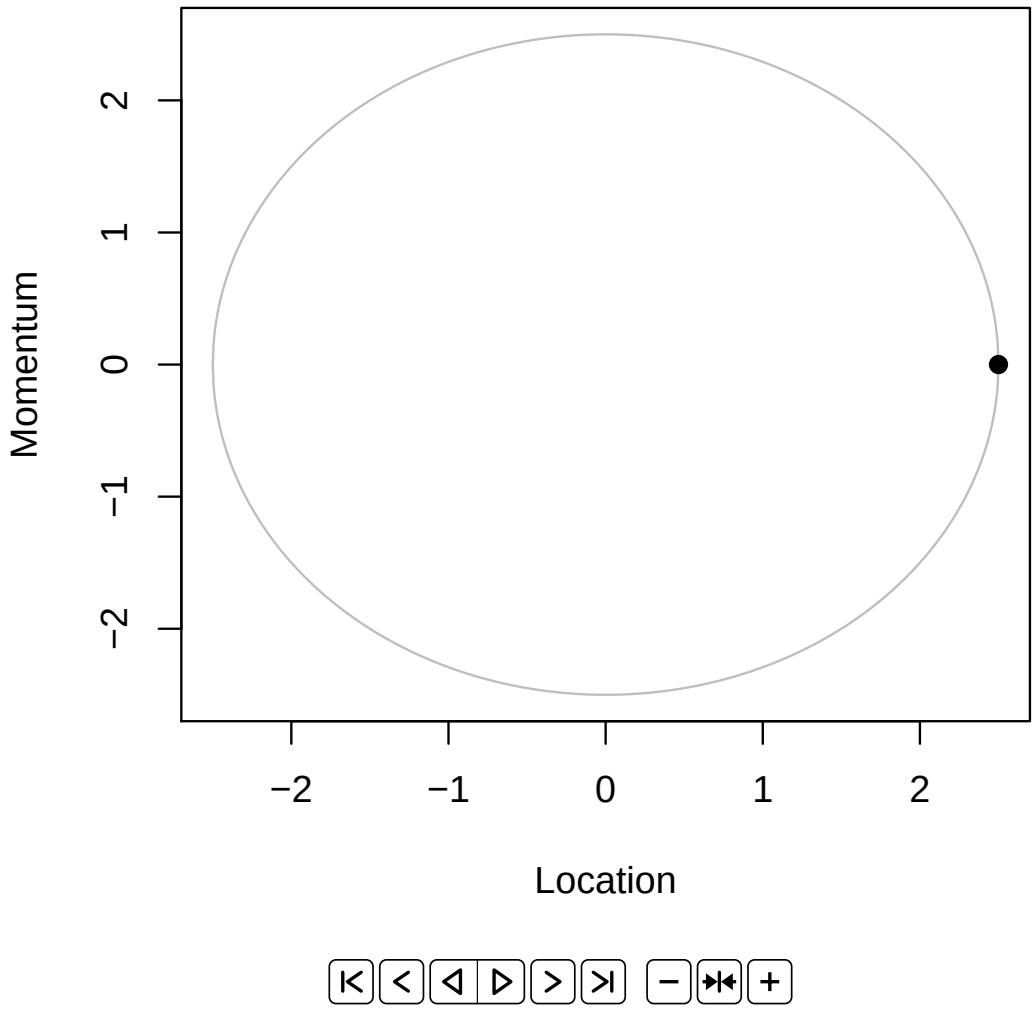
Leap-frog simulator

```
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", q, and "momentum", p, and so defines a joint distribution for them, via

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

where Z is the normalizing constant.
If $H(q,p) = U(q) + K(p)$, the joint density is

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

If we are interested in a posterior distribution, we set $q = \theta$ and

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

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

A reversible simulation 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 (θ', ω') for the same e and L, you will end up at (θ, ω).

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, but so long as $p(\omega) = p(-\omega)$ this will not affect our acceptance probability.

Volume preserving results in perfect acceptance

Recall that we accept with probability $\min\{1, \rho(\theta^{(i)}, \theta^*)\}$ where

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

Volume is preserved if

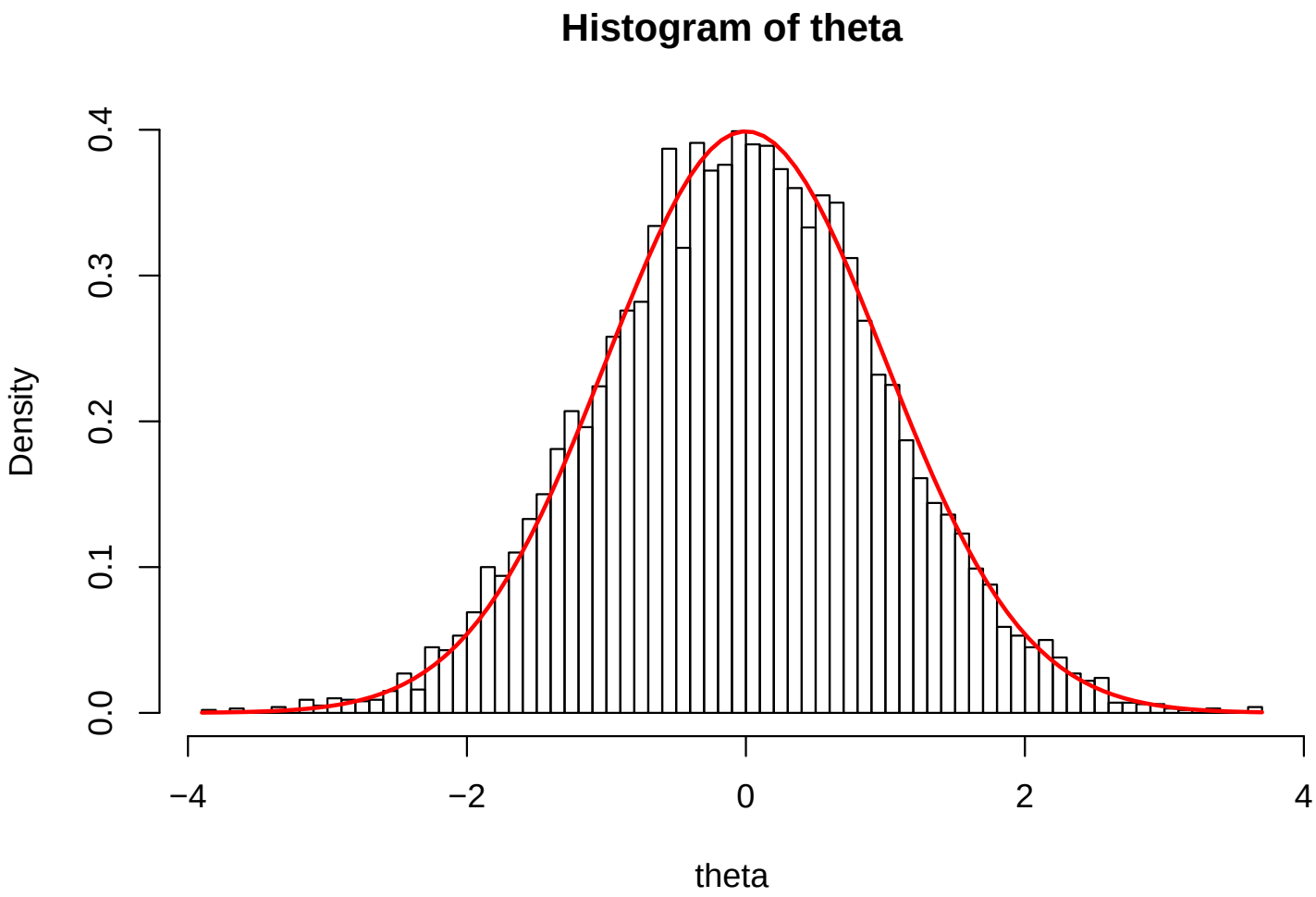
$$p(\theta^{(i)}|y)p(\omega^{(i)}) = p(\theta^*|y)p(\omega^*) \implies \frac{p(\theta^*|y)}{p(\theta^{(i)}|y)} \frac{p(\omega^*)}{p(\omega^{(i)})} = 1$$

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, epsilon, L, current_q) {
  q = current_q
  p = rnorm(length(q),0,1)
  current_p = p

  p = p-epsilon*grad_U(q)/2

  for (i in 1:L) {
    q = q+epsilon*p
    if (i!=L) p = p -epsilon * grad_U(q)
  }
  p = p-epsilon * grad_U(q)/2

  p = -p

  current_U = U(current_q)
  current_K = sum(current_p^2)/2
  proposed_U = U(q)
  proposed_K = sum(p^2)/2

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

```
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

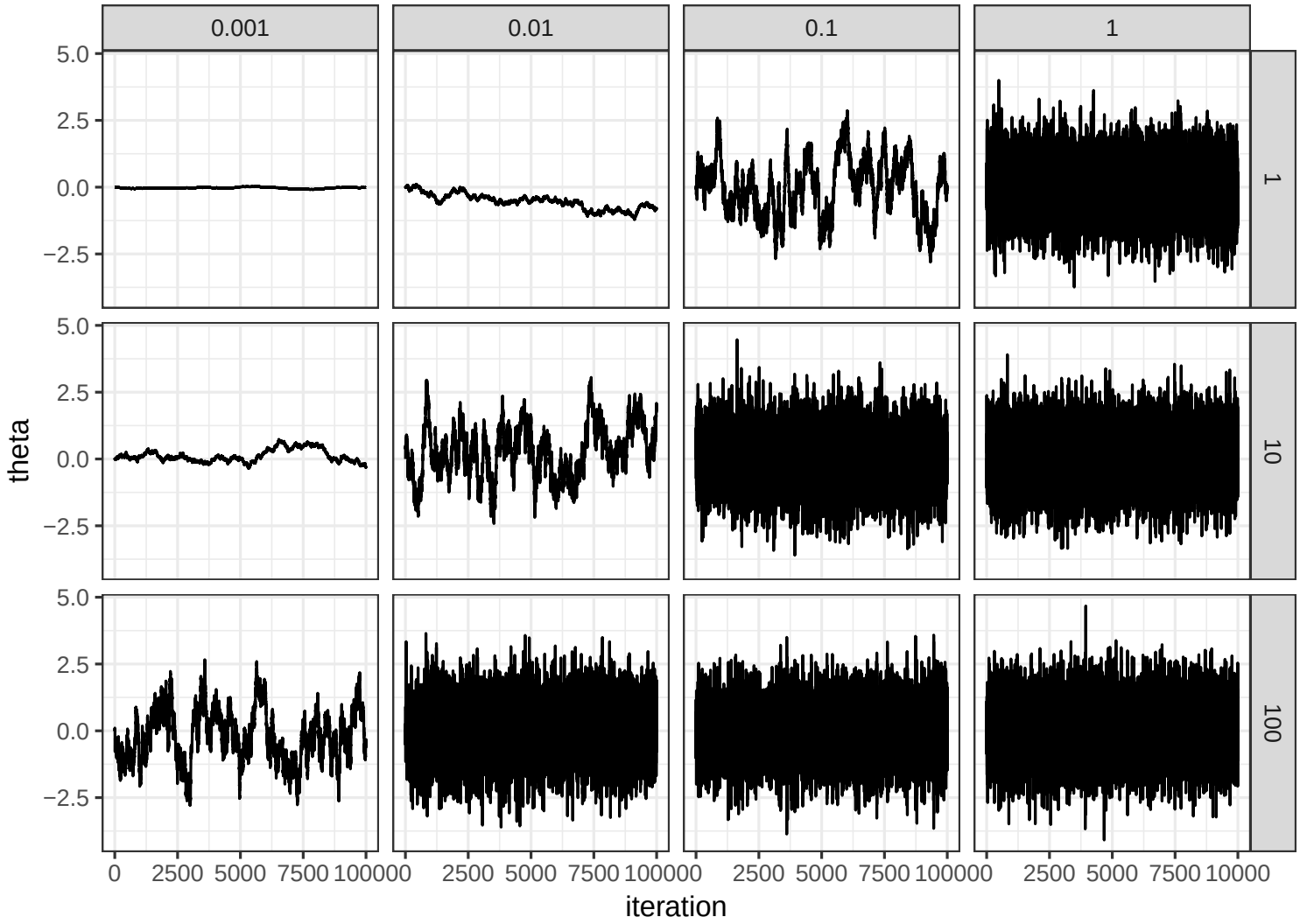
There are three tuning parameters:

- 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^seq(-3,0,by=1), L=10^seq(0,2))
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)))
})
```


0.001
0.01
0.1
1
1
10
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theta
5.0
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2500
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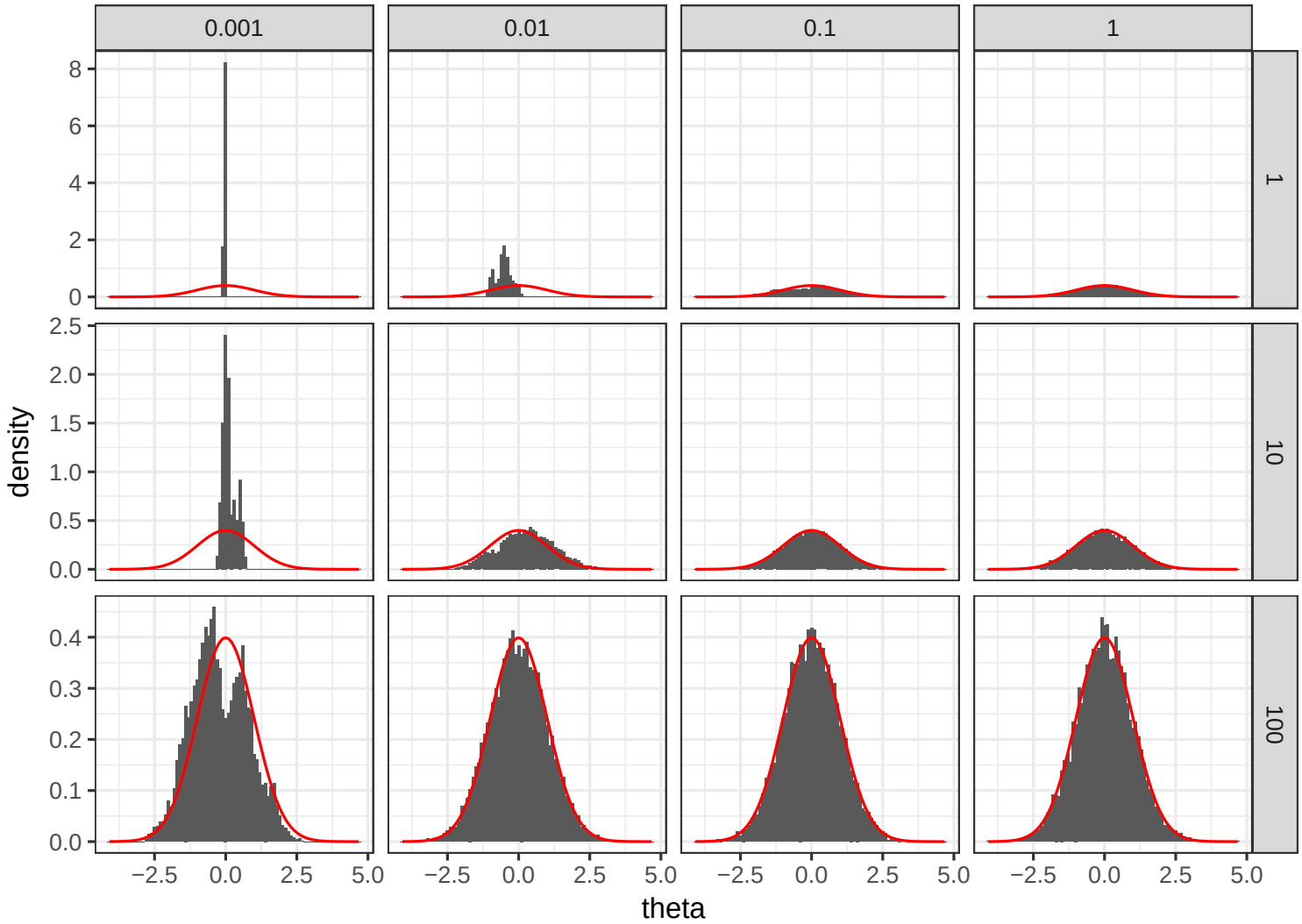
10000
iteration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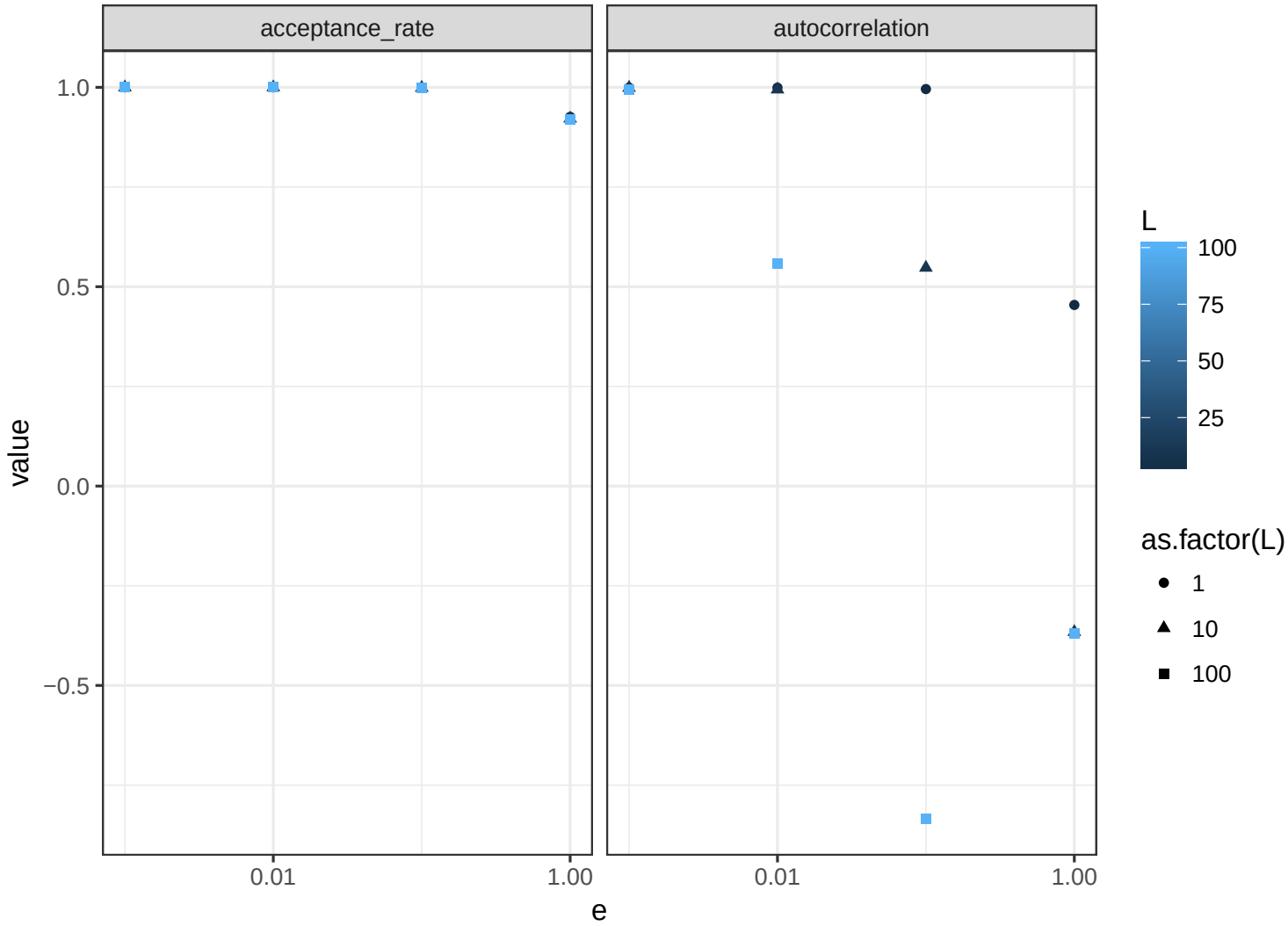
acceptance_rate
autocorrelation
value
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0.5
0.0
−0.5
0.01
1.00
0.01
1.00
e
L
100
75
50
25
as.factor(L)
1
10
100

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 $\mathbb{R}^d$).