project_report

June 1, 2023

1 Monte Carlo Methods Project

1.1 Getting started

To run the code, first install Julia:

1. Visit https://julialang.org/downloads/ and select the installer for your system (I used 1.8.3, but probably 1.9.0 will work just as well). If you're on Linux, run:

```
wget https://julialang-s3.julialang.org/bin/linux/x64/1.8/julia-1.8.3-linux-x86_64.tar.gz
tar zxvf julia-1.8.3-linux-x86_64.tar.gz
```

2. On Linux, that's all you have to do. You can choose to make the `julia` executable more accessible by, e.g., opening `~/.bashrc` and adding the line:

```
export PATH="$PATH:/path/to/<Julia directory>/bin"
```

3. Make sure to start a new terminal or run `source ~/.bashrc` afterwards.

Consequently, you want to install the relevant packages:

1. Move one level above the current directory (the current directory is the one that contains this file) and activate Julia:

```
cd ..
julia
```

2. Inside Julia, change to the Pkg mode by typing `]`. In there, you want to activate the project toml file and instantiate the project. This will install all necessary packages and precompile them.

```
]
activate Project
instantiate
```

[ ]:
```
using LinearAlgebra
using Distributions
using Plots
```

General note: It was not quite clear to me whether the starting values should be returned by the sampling algorithms, or discarded. Either way, I don't think it matters much, but I decided to be prudent and discard the starting values.

2 Exercise (a)

[ ]:
```
function quadraticpotential_grad(q)
    q
end

function leapfrog(q0, p0, tau, l, mass, potential_grad::Function)
    # Determine dimensionality
    d = length(q0)

    # Also accomodate initial values
    qs = [Vector{Float64}(undef, d) for _ = 1:(l+1)]
    ps = [Vector{Float64}(undef, d) for _ = 1:(l+1)]

    qs[1] = q0
    ps[1] = p0

    for i = 2:(l+1)
        p_half = ps[i - 1] .- tau / 2 .* potential_grad(qs[i - 1])
        qs[i] = qs[i - 1] .+ tau * inv(mass) * p_half
        ps[i] = p_half .- tau / 2 .* potential_grad(qs[i])
    end

    # Discard initial value
    (qs[2:(l+1)], ps[2:(l+1)])
end
```

```
leapfrog (generic function with 1 method)
```

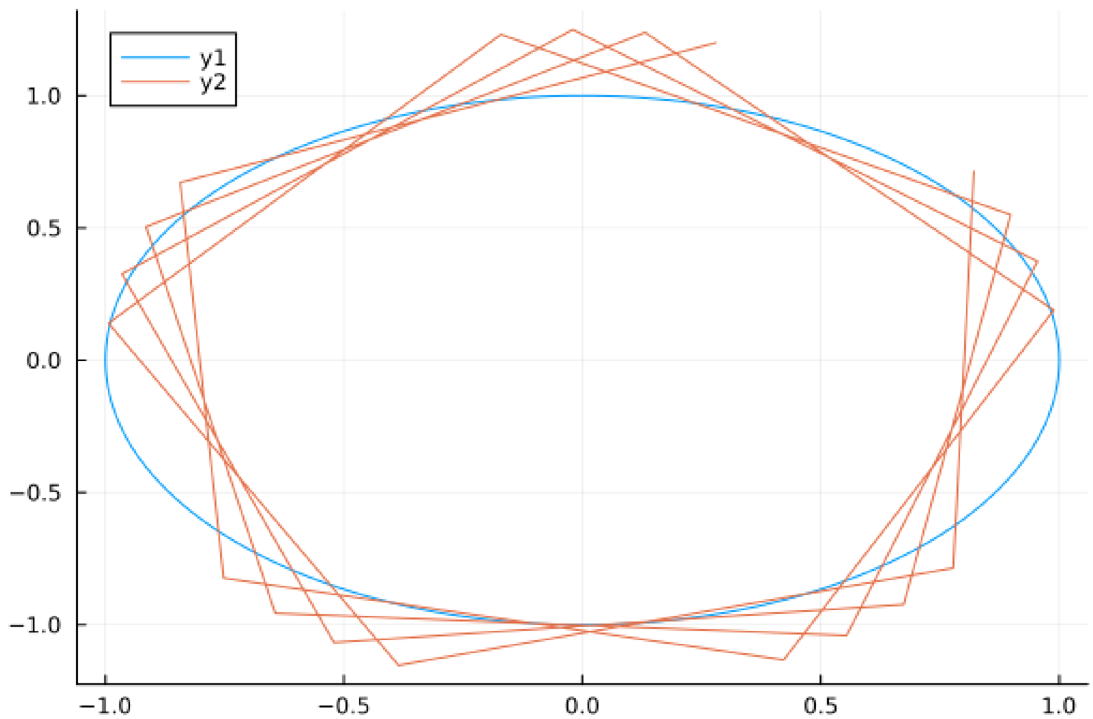
3 Exercise (b)

[ ]:
```
q0 = [0.]
p0 = [1.]
tau = 1.2
l = 20
mass = [1.;;]

(ps1, qs1) = leapfrog(q0, p0, tau, l, mass, quadraticpotential_grad)

tau = 0.3
l = 80

(ps2, qs2) = leapfrog(q0, p0, tau, l, mass, quadraticpotential_grad);
```

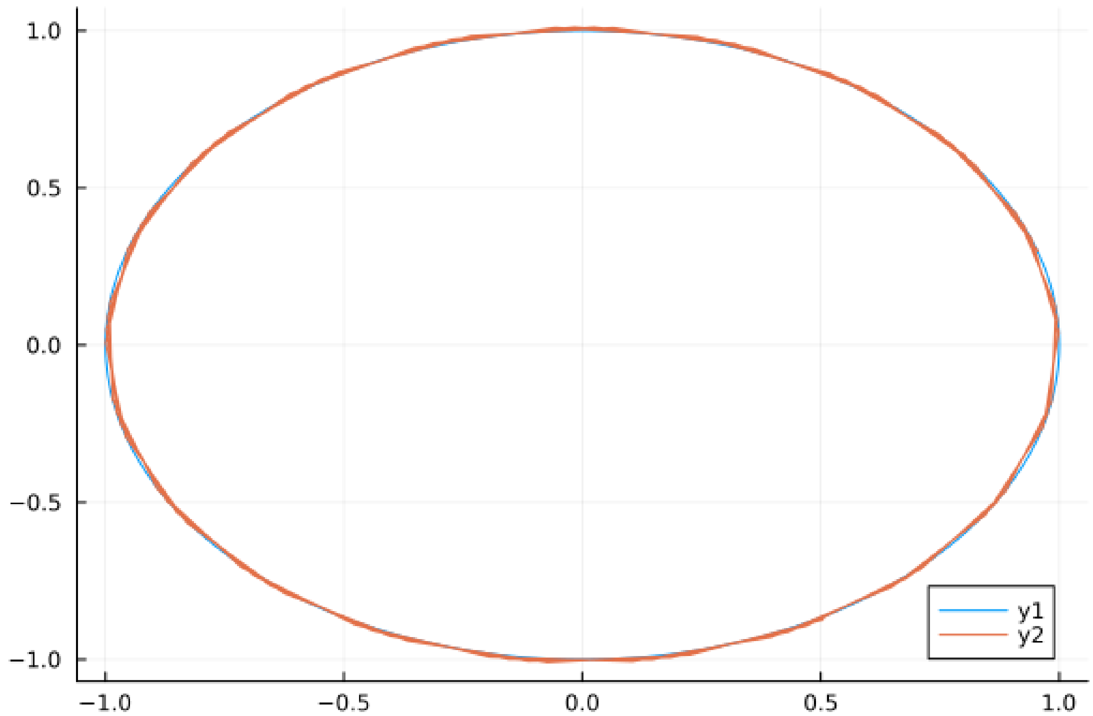
[ ]:
```
qs1_flat = [v[1] for v in qs1]
ps1_flat = [v[1] for v in ps1]
```

```
qs2_flat = [v[1] for v in qs2]
ps2_flat = [v[1] for v in ps2];
```

[ ]:
```
t = collect(0:0.01:2 )
q_exact = -cos.(t .+  /2)
p_exact = sin.(t .+  /2)

plot(q_exact, p_exact)
plot!(qs1_flat, ps1_flat)
```



[ ]:
```
plot(q_exact, p_exact)
plot!(qs2_flat, ps2_flat)
```



4 Exercise (c)

Substituting Equation (4) into (7), and then using Equation (8), we get:

$$\begin{aligned}\pi(\mathbf{q},\mathbf{p}) &\propto \exp\left(-H(\mathbf{q},\mathbf{p})\right)\\ &\propto e^{-U(\mathbf{q})-K(\mathbf{p})}\\ &\propto e^{--ln(\pi(\mathbf{q}))}e^{-\frac{1}{2}\mathbf{p}^T M^{-1}\mathbf{p}}\\ &\propto \pi(\mathbf{q})e^{-\frac{1}{2}\mathbf{p}^T M^{-1}\mathbf{p}}.\end{aligned}$$

If we fix $\mathbf{p}$, we can treat it as a constant:

$$\begin{aligned}\pi(\mathbf{q}\mid\mathbf{p}) &\propto \pi(\mathbf{q})e^{-\frac{1}{2}\mathbf{p}^T M^{-1}\mathbf{p}}\\ &\propto \pi(\mathbf{q}).\end{aligned}$$

This shows that sampling from $\pi(\mathbf{q},\mathbf{p})$ is equivalent to sampling from $\pi(\mathbf{q})$ if $\mathbf{p}$ is fixed.

5 Exercise (d)

Fixing $\mathbf{q}$ to specify a pdf for $\mathbf{p}$ yields:

$$\begin{aligned}\pi(\mathbf{p} \mid \mathbf{q}) &\propto \pi(\mathbf{q}) e^{-\frac{1}{2}\mathbf{p}^T M^{-1}\mathbf{p}} \\ &\propto e^{-\frac{1}{2}\mathbf{p}^T M^{-1}\mathbf{p}} \\ &\propto (2\pi)^{-d/2} \det{(M)}^{-1/2} e^{-\frac{1}{2}\mathbf{p}^T M^{-1}\mathbf{p}}.\end{aligned}$$

In other words, $\pi(\mathbf{p} \mid \mathbf{q})$ is equal to a 0-mean multivariate Gaussian pdf up to a normalising constant. M can be interpreted as the covariance matrix of that Gaussian.

6 Exercise (e)

$-H(\mathbf{q}^*, \mathbf{p}^*) + H(\mathbf{q}, \mathbf{p})$ can be interpreted as $\frac{\Delta H}{\Delta t}$. We have seen above that with an exact trajectory, the Hamiltonian is conserved: $\frac{dH}{dt} = 0$. Under this condition, the acceptance probability becomes:

$$\begin{aligned}\alpha &= \min\{1, \exp\left(-H(\mathbf{q}^*, \mathbf{p}^*) + H(\mathbf{q}, \mathbf{p})\right)\} \\ &= \min\{1, \exp(0)\} \\ &= 1.\end{aligned}$$

This means that using an approach that approximates the trajectory well would lead to acceptance probabilities close to 1.

7 Exercise (f)

[ ]:
```
function quadraticpotential(q)
    0.5 * q' * q
end

function hamiltonian(q, p, mass, potential::Function)
    potential(q) + 0.5 * p' * inv(mass) * p
end

function hmc(n, q0, tau_dist, l, potential::Function, potential_grad::Function)
    # Determine dimensionality
    d = length(q0)

    # Also accomodate initial values
    qs = [Vector{Float64}(undef, d) for _ = 1:(n+1)]
    ps = [Vector{Float64}(undef, d) for _ = 1:(n+1)]

    # Julia can infer the size of I from the mathematical context
    mass = I
    norm = MvNormal(zeros(Float64, d), mass)

    qs[1] = q0
```

```
    for t = 2:(n+1)
        ps[t - 1] = vec(rand(norm, 1))

        tau = rand(tau_dist, 1)[1]
        # Note that qs_star has a different dimensionality (l) than qs (n)
        (qs_star, ps_star) = leapfrog(qs[t - 1], ps[t - 1], tau, l, mass,␣
↪potential_grad)
        q_star = qs_star[l]
        p_star = ps_star[l]

        h_prev = hamiltonian(qs[t - 1], ps[t - 1], mass, potential)
        h_star = hamiltonian(q_star, p_star, mass, potential)

        alpha = min(1, exp(h_prev - h_star))

        if rand() < alpha
            qs[t] = q_star
            ps[t] = p_star
        else
            qs[t] = qs[t - 1]
            ps[t] = ps[t - 1]
        end
    end

    (qs[2:(n+1)], ps[2:(n+1)])
end
```

```
hmc (generic function with 1 method)
```

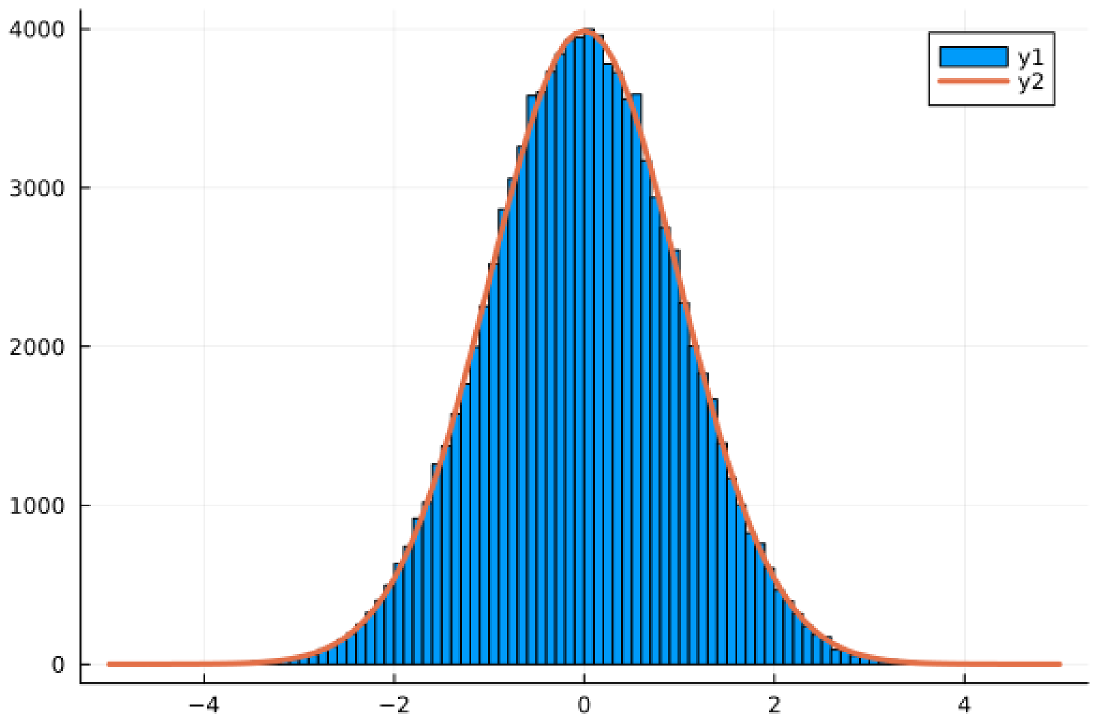
Testing with the quadratic potential and its gradient. Since we are not applying a -log to to the potential, we are essentially sampling from:

$$\begin{aligned}
\pi(\mathbf{q} \mid \mathbf{p}) &\propto e^{-U(\mathbf{q})-K(\mathbf{p})} \\
&\propto e^{-U(\mathbf{q})} \\
&\propto e^{-\frac{1}{2}\mathbf{q}^T\mathbf{q}},
\end{aligned}$$

which is proportional to a multivariate normal pdf with mean 0 and covariance matrix I. In other words, we should get a normal distribution if we set $d = 1$, which the histogram below shows to be the case.

[ ]:
```
tau_dist = Uniform(0.5, 1.5)
samples, _ = hmc(100000, q0, tau_dist, l, quadraticpotential,␣
↪quadraticpotential_grad);
```

[ ]:
```
samples_flat = [s[1] for s in samples]
histogram(samples_flat)

x = -5:0.1:5
plot!(x, pdf.(Normal(0, 1), x) .* 1e4, linewidth = 3)
```



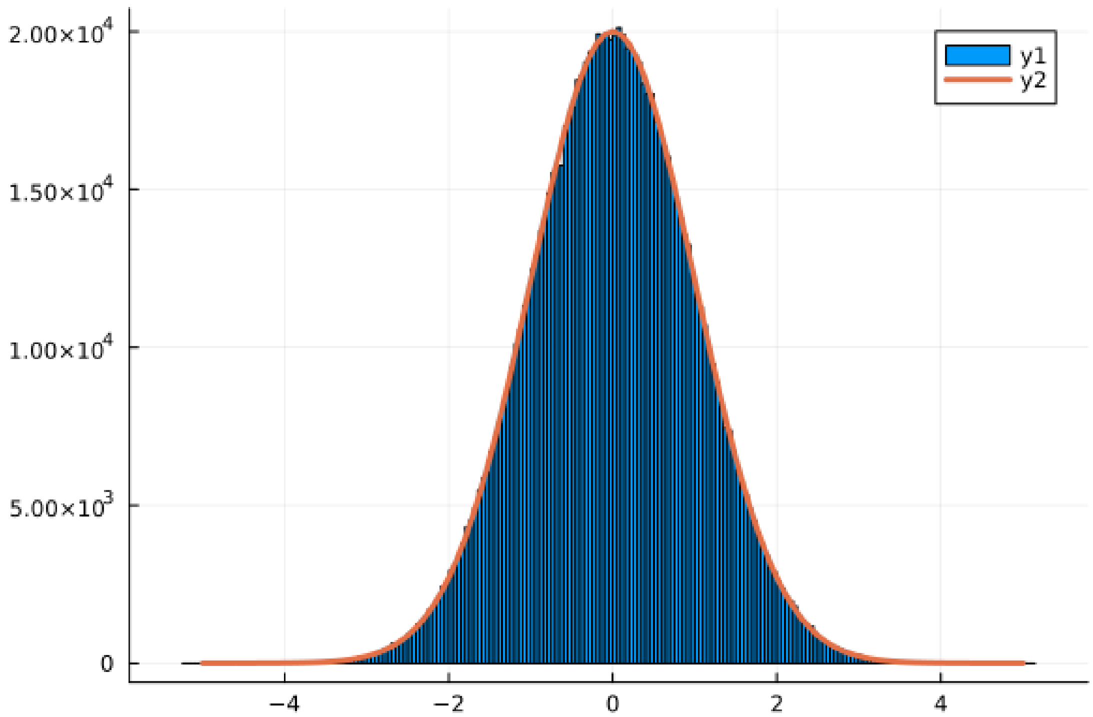
8 Exercise (g)

[ ]:
```
function rw_mh(n, start, prop_dist, target::Function)
    d = length(start)

    samples = [Vector{Float64}(undef, d) for _ = 1:(n+1)]
    samples[1] = start

    for i = 2:(n+1)
        sample_prop = vec(rand(prop_dist, 1)) + samples[i - 1]

        dens_prev = target(samples[i - 1])
        dens_prop = target(sample_prop)
        alpha = min(1, dens_prop / dens_prev)

        if rand() < alpha
```

```
            samples[i] = sample_prop
        else
            samples[i] = samples[i - 1]
        end
    end

    samples[2:(n+1)]
end
```

rw_mh (generic function with 1 method)

```
[ ]: target(x) = exp(-quadraticpotential(x))
samples = rw_mh(1000000, [0.], MvNormal(zeros(1), I), target)
histogram([s[1] for s in samples])

x = -5:0.1:5
plot!(x, target.(x) .* 2e4, linewidth = 3)
```



9 Exercise (h)

[ ]:
```
function rand_sigma_mh(n, start, sigma_dist, target::Function)
    mh_samples = [Vector{Float64}(undef, d) for _ = 1:(n+1)]
    mh_samples[1] = start

    mu = zeros(size(start))

    for i = 2:(n+1)
        sigma = rand(sigma_dist, 1)[1]
        prop_dist = MvNormal(mu, sigma * I)

        mh_samples[i] = rw_mh(1, mh_samples[i - 1], prop_dist, target)[1]
    end

    mh_samples[2:(n+1)]
end
```

```
rand_sigma_mh (generic function with 1 method)
```

To be able to use Hamiltonian Monte Carlo, we first need to find the gradient $\nabla_{\mathbf{q}} U$. Since

$$\nabla_{\mathbf{q}} U = \begin{pmatrix} \frac{\partial U}{\partial q_1} \\ \vdots \\ \frac{\partial U}{\partial q_d} \end{pmatrix},$$

we need to find $\frac{\partial U}{\partial q_i}$, where $i = 1, \ldots, d$. Because we want to sample from a multivariate normal, we get the -log of its pdf:

$$\begin{aligned} \frac{\partial U}{\partial q_i} &= \frac{\partial}{\partial q_i} \left[-\log\left((2\pi)^{-\frac{d}{2}} \det(\Sigma)^{-\frac{1}{2}} e^{-\frac{1}{2}\mathbf{q}^T \Sigma^{-1} \mathbf{q}} \right) \right] \\ &= \frac{\partial}{\partial q_i} \left[-\left(\log\left((2\pi)^{-\frac{d}{2}} \det(\Sigma)^{-\frac{1}{2}} \right) + \log\left(e^{-\frac{1}{2}\mathbf{q}^T \Sigma^{-1} \mathbf{q}} \right) \right) \right] \\ &= \frac{\partial}{\partial q_i} \left[\frac{1}{2} \mathbf{q}^T \Sigma^{-1} \mathbf{q} \right]. \end{aligned}$$

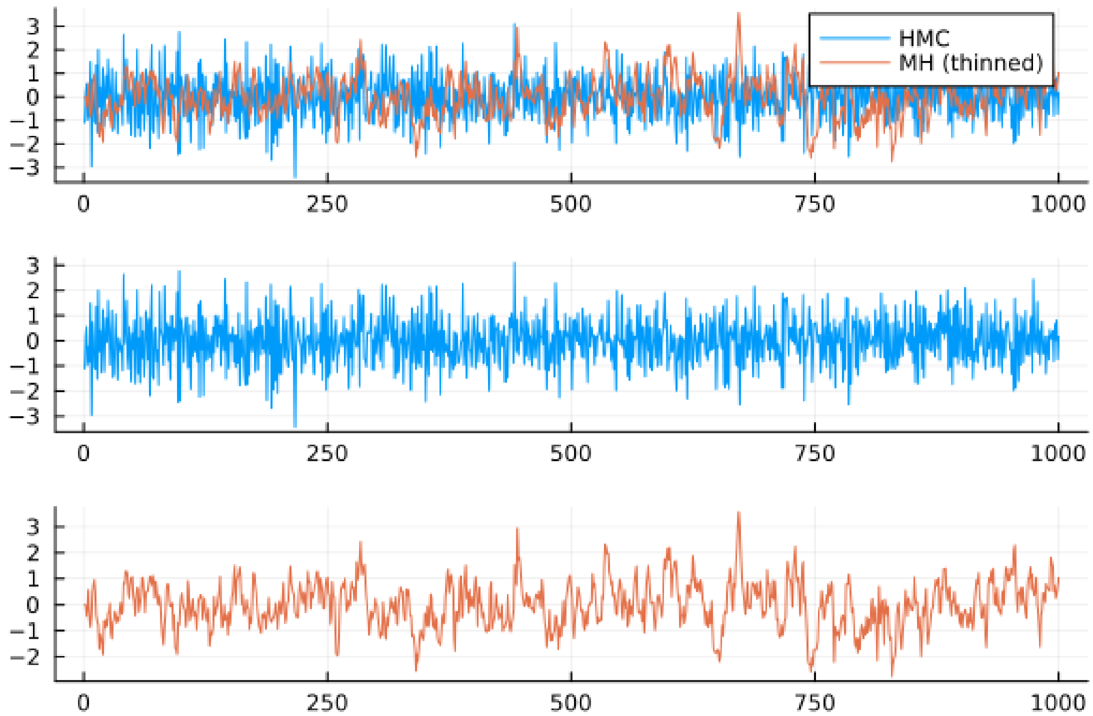
Σ is diagonal, so its inverse can be found by taking the reciprocals of its diagonal values:

$$
\begin{aligned}
\frac{\partial U}{\partial q_i} &= \frac{\partial}{\partial q_i}\left[\frac{1}{2}\mathbf{q}^T \begin{pmatrix} \frac{1}{\sigma_1} & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \frac{1}{\sigma_d} \end{pmatrix} \mathbf{q}\right] \\
&= \frac{\partial}{\partial q_i}\left[\frac{1}{2}\mathbf{q}^T \begin{pmatrix} \frac{1}{\sigma_1} q_1 \\ \vdots \\ \frac{1}{\sigma_d} q_d \end{pmatrix}\right] \\
&= \frac{\partial}{\partial q_i}\left[\frac{1}{2}\left(\frac{1}{\sigma_1} q_1^2 + \cdots + q_d^2\right)\right] \\
&= \frac{1}{\sigma_i} q_i.
\end{aligned}
$$

[ ]:
```
sigmas = collect(0.01:0.01:1)
Σ = Diagonal(sigmas)
d = size(Σ, 1)
  = zeros(d)
target(x) = pdf(MvNormal( , Σ), x)

n = 1000
l = 150
tau_dist = Uniform(0.0104, 0.0156)
potential(x) = -log(target(x))
potential_grad(x) = @. (1 / sigmas) * x
samples_hmc, _ = hmc(n,  , tau_dist, l, potential, potential_grad)

n = 150000
sigma_dist = Uniform(0.0176, 0.0264)
samples_mh = rand_sigma_mh(n,  , sigma_dist, target)
samples_mh_thinned = samples_mh[1:150:length(samples_mh)];
```

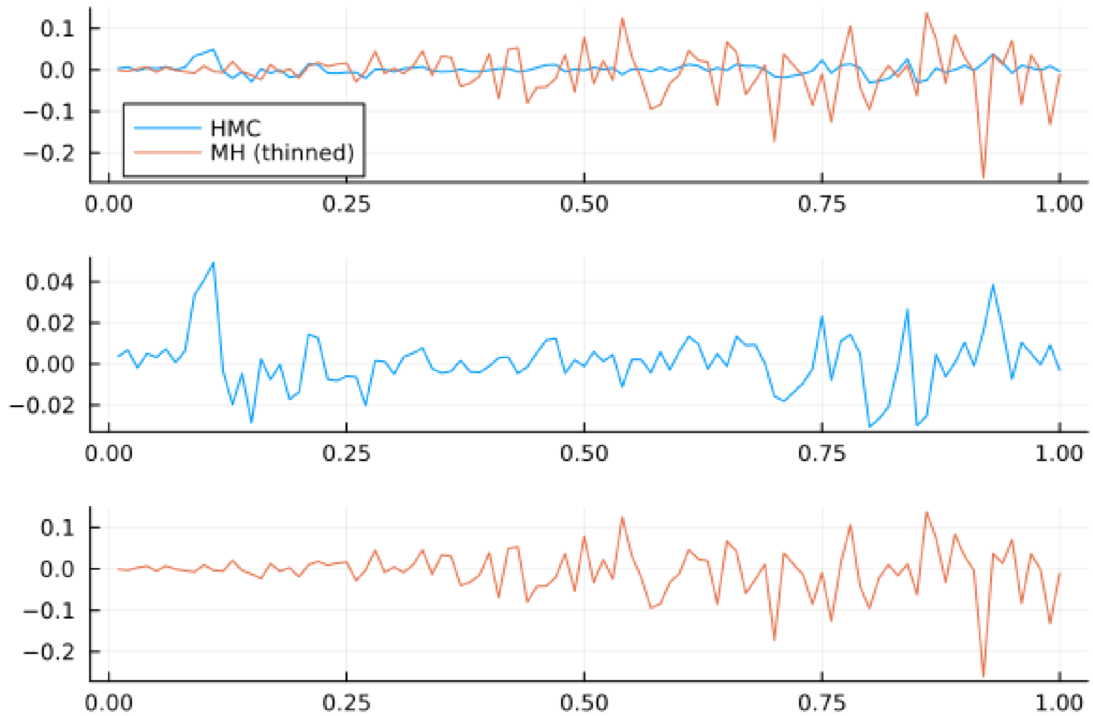
Plotting the HMC and thinned MH samples (first on top of each other, then separately) shows that the MH chain moves/mixes much slower than the HMC one. In other words, there seems to be more autocorrelation in the MH samples.

[ ]:
```
last_comp_hmc = [v[d] for v in samples_hmc]
last_comp_mh_th = [v[d] for v in samples_mh_thinned]

plot(last_comp_hmc, labels = "HMC")
p1 = plot!(last_comp_mh_th, labels = "MH (thinned)")

p2 = plot(last_comp_hmc, legend = false)

p3 = plot(last_comp_mh_th, color = 2, legend = false)

plot(p1, p2, p3, layout = (3, 1))
```



Plotting the sample variation over the component standard deviations, we see a fairly constant error for the HMC sampler (except for a little dip at the very end), while for the MH sampler, the error seems to increase with the standard deviation.

[ ]:
```
# Turns the vector of vectors inside-out (components outside, samples inside)
comps_hmc = [[v[i] for v in samples_hmc] for i = 1:d]
means_hmc = mean.(comps_hmc)
plot(sigmas, means_hmc, labels = "HMC")

comps_mh = [[v[i] for v in samples_mh] for i = 1:d]
means_mh = mean.(comps_mh)
p1 = plot!(sigmas, means_mh, labels = "MH (thinned)")

p2 = plot(sigmas, means_hmc, legend = false)

p3 = plot(sigmas, means_mh, color = 2, legend = false)

plot(p1, p2, p3, layout = (3, 1))
```



HMC
MH (thinned)
0.1
0.0
−0.1
−0.2
0.00
0.25
0.50
0.75
1.00
0.04
0.02
0.00
−0.02