1 Metropolis–Hastings MCMC

X **and** x state (possibly multivariate)

$f_X(x)$ target density (we want to sample from), that we can't compute

$\pi(x)$ density of x up to a constant, that we can

$q(\cdot|\cdot)$ proposal density

$$f_X(x) = \frac{\pi(x)}{\int \pi(x')dx'}$$

1. Starting with $x^{(0)}$.
2. Propose $x^\star \sim q(x^\star|x^{(t)})$.
3. Compute $\alpha = \min\left(1, \frac{\pi(x^\star)}{\pi(x^{(t)})} \times \frac{q(x^{(t)}|x^\star)}{q(x^\star|x^{(t)})}\right)$.
4. With probability α, make $x^{(t+1)} = x^\star$, otherwise $x^{(t+1)} = x^{(t)}$.
5. Continue from 2 for a while.

2 Parallel Tempering MCMC

T **and** τ "temperature" variables.

$f_{X,T}(x,\tau)$ augmented target density, in particular $f_{X,T}(x,1) \equiv f_X(x)$

$$f_{X,T}(x,\tau) = \frac{\pi(x)^{1/\tau}}{\int\int \pi(x')^{1/\tau'}dx'd\tau'}$$

1. Starting with $(x^{(0,1)}, \tau^{(0,1)})$ and $(x^{(0,2)}, \tau^{(0,2)})$.
2. For $i = 1, 2$
   (a) Propose $x^\star \sim q(x^\star|x^{(t,i)})$.
   (b) Compute $\alpha = \min\left(1, \frac{\pi(x^\star)^{1/\tau_i}}{\pi(x^{(t,i)})^{1/\tau_i}} \times \frac{q(x^{(t,i)}|x^\star)}{q(x^\star|x^{(t,i)})}\right)$.
   (c) With probability α, make $x^{(t+1,i)} = x^\star$, otherwise $x^{(t+1,i)} = x^{(t,i)}$.
3. Propose $(x^{\star,1}, \tau^{\star,1}) = (x^{(t,1)}, \tau^{(t,2)})$ and $(x^{\star,2}, \tau^{\star,2}) = (x^{(t,2)}, \tau^{(t,1)})$.

4. Compute $\alpha_\tau = \min\left(1, \frac{\pi(x^{(t,1)})^{1/\tau^{(t,2)}} \times \pi(x^{(t,2)})^{\tau^{(t,1)}}}{\pi(x^{(t,1)})^{1/\tau^{(t,1)}} \times \pi(x^{(t,2)})^{1/\tau^{(t,2)}}}\right)$.

5. With probability α_τ, make $(x^{(t+1,1)}, \tau^{(t+1,1)}) = (x^{(t,1)}, \tau^{(t,2)})$ and $(x^{(t+1,2)}, \tau^{(t+1,2)}) = (x^{(t,2)}, \tau^{(t,1)})$, otherwise copy old configurations.

6. Continue from 2 for a while.

7. Take those samples $(x^{(t)}, \tau^{(t)})$ where $\tau^{(t)} = 1$.

3 Application to ERGM

3.1 Ordinary MCMC

In an ERGM, the numerator is:

$$\pi(x) = e^{\eta(\theta)\cdot g(x)}$$

Then, M–H acceptance is

$$\begin{aligned}
\alpha &= \min\left(1, \frac{\pi(x^\star)}{\pi(x^{(t)})} \times \frac{q(x^{(t)}|x^\star)}{q(x^\star|x^{(t)})}\right) \\
&= \min\left(1, \frac{e^{\eta(\theta)\cdot g(x^\star)}}{e^{\eta(\theta)\cdot g(x^{(t)})}} \times \frac{q(x^{(t)}|x^\star)}{q(x^\star|x^{(t)})}\right) \\
&= \min\left(1, e^{\eta(\theta)\cdot g(x^\star) - \eta(\theta)\cdot g(x^{(t)})} \times \frac{q(x^{(t)}|x^\star)}{q(x^\star|x^{(t)})}\right) \\
&= \min\left(1, e^{\eta(\theta)\cdot\{g(x^\star) - g(x^{(t)})\}} \times \frac{q(x^{(t)}|x^\star)}{q(x^\star|x^{(t)})}\right) \\
&= \exp\min\left(0, \eta(\theta)\cdot\{g(x^\star) - g(x^{(t)})\} + \log\frac{q(x^{(t)}|x^\star)}{q(x^\star|x^{(t)})}\right)
\end{aligned}$$

3.2 Parallel tempering MCMC

With tempering in effect,

$$\pi(x)^{1/\tau} = (e^{\eta(\theta)\cdot g(x)})^{1/\tau} = e^{\eta(\theta)\cdot g(x)/\tau} = e^{\{\eta(\theta)/\tau\}\cdot g(x)}$$

$$\alpha_\tau = \min\left(1, e^{\{\eta(\theta)/\tau\}\cdot\{g(x^\star) - g(x^{(t)})\}} \times \frac{q(x^{(t)}|x^\star)}{q(x^\star|x^{(t)})}\right)$$