

CPSC 535

Metropolis-Hastings

AD

March 2007

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Gibbs Sampler

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- For $k = 1 : p$

- Sample $\theta_k^{(i)} \sim \pi \left(\theta_k | \theta_{-k}^{(i)} \right)$ where

$$\theta_{-k}^{(i)} = \left(\theta_1^{(i)}, \dots, \theta_{k-1}^{(i)}, \theta_{k+1}^{(i-1)}, \dots, \theta_p^{(i-1)} \right).$$

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- For many complex models, it is impossible to sample from several of these “full” conditional distributions.
- Even if it is possible to implement the Gibbs sampler, the algorithm might be very inefficient because the variables are very correlated or sampling from the full conditionals is extremely expensive/inefficient.

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- This can be interpreted as the basis of all MCMC algorithm: It provides a generic way to build a Markov kernel admitting $\pi(\theta)$ as an invariant distribution.
- The Metropolis algorithm was named the “Top algorithm of the 20th century” by computer scientists, mathematicians, physicists.

- Introduce a proposal distribution/kernel $q(\theta, \theta')$, i.e.

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- The basic idea of the MH algorithm is to propose a new candidate θ' based on the current state of the Markov chain θ .
- We only accept this algorithm with respect to a probability $\alpha(\theta, \theta')$ which ensures that the invariant distribution of the transition kernel is the target distribution $\pi(\theta)$.

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 - Sample $\theta^* \sim q(\theta^{(i-1)}, \theta^*)$ and compute

$$\alpha(\theta^{(i-1)}, \theta^*) = \min \left(1, \frac{\pi(\theta^*) q(\theta^*, \theta^{(i-1)})}{\pi(\theta^{(i-1)}) q(\theta^{(i-1)}, \theta^*)} \right).$$

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- With probability $\alpha(\theta^{(i-1)}, \theta^*)$, set $\theta^{(i)} = \theta^*$; otherwise set $\theta^{(i)} = \theta^{(i-1)}$.

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- This algorithm is extremely general: $q(\theta, \theta')$ can be any proposal distribution. So in practice, we can select it so that it is easy to sample from it.
- There is much more freedom than in the Gibbs sampler where the proposal distributions are fixed.

Random Walk Metropolis

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- The distribution $f(z)$ is the distribution of the random walk increments Z and

$$q(\theta, \theta') = f(\theta' - \theta) \Rightarrow \alpha(\theta, \theta') = \min \left(1, \frac{\pi(\theta') f(\theta - \theta')}{\pi(\theta) f(\theta' - \theta)} \right).$$

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- If $f(\theta' - \theta) = f(\theta - \theta')$ - e.g. $Z \sim \mathcal{N}(0, \Sigma)$ - then

$$\alpha(\theta, \theta') = \min \left(1, \frac{\pi(\theta')}{\pi(\theta)} \right)$$

Independent Metropolis-Hastings

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- In this case, the acceptance probability is given by

$$\alpha(\theta, \theta') = \min\left(1, \frac{\pi(\theta') q(\theta)}{\pi(\theta) q(\theta')}\right) = \min\left(1, \frac{\pi^*(\theta') q^*(\theta)}{q^*(\theta') \pi^*(\theta)}\right)$$

where π^* and q^* are unnormalized versions of π and q .

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where π^* and q^* are unnormalized versions of π and q .

- The ratio $\pi^*(\theta) / q^*(\theta)$ appearing in the Accept/Reject and Importance Sampling methods also reappears here.

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 - $\pi(\theta)$ is the invariant distribution of the Markov kernel associated to the MH algorithm.
 - The Markov chain is irreducible; i.e. one can reach any set A such that $\pi(A) > 0$.
 - The Markov chain is aperiodic; i.e. one does not visit in a periodic way the state-space.

Invariance of the MH kernel

- The transition kernel associated to the MH algorithm can be rewritten as

$$K(\theta, \theta') = \alpha(\theta, \theta') q(\theta, \theta') + \underbrace{\left(1 - \int \alpha(\theta, u) q(\theta, u) du\right)}_{\text{rejection probability}} \delta_{\theta}(\theta')$$

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- **Remark:** This is a loose notation for

$$K(\theta, d\theta') = \alpha(\theta, \theta') q(\theta, \theta') d\theta' + \left(1 - \int \alpha(\theta, u) q(\theta, u) du\right) \delta_{\theta}(d\theta').$$

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- Clearly we have

$$\begin{aligned} \int K(\theta, \theta') d\theta' &= \int \alpha(\theta, \theta') q(\theta, \theta') d\theta' \\ &\quad + \left(1 - \int \alpha(\theta, u) q(\theta, u) du\right) \int \delta_{\theta}(\theta') d\theta' \\ &= 1. \end{aligned}$$

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- Note that this condition is satisfied if the *reversibility property* is satisfied: For all θ, θ'

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- Indeed the reversibility condition implies that

$$\begin{aligned} \int \pi(\theta) K(\theta, \theta') d\theta &= \int \pi(\theta') K(\theta', \theta) d\theta \\ &= \pi(\theta') \int K(\theta', \theta) d\theta \\ &= \pi(\theta') \end{aligned}$$

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- The deterministic scan Gibbs sampler is not π -reversible as

$$\pi(\theta_1, \theta_2) \pi(\theta'_2 | \theta_1) \pi(\theta'_1 | \theta'_2) \neq \pi(\theta'_1, \theta'_2) \pi(\theta_2 | \theta'_1) \pi(\theta'_2 | \theta'_1).$$

- By definition of the kernel, we have

$$\begin{aligned} \pi(\theta) K(\theta, \theta') &= \pi(\theta) \alpha(\theta, \theta') q(\theta, \theta') \\ &+ \left(1 - \int \alpha(\theta, u) q(\theta, u) du\right) \delta_{\theta}(\theta') \pi(\theta). \end{aligned}$$

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- Then

$$\begin{aligned} \pi(\theta) \alpha(\theta, \theta') q(\theta, \theta') &= \pi(\theta) \min\left(1, \frac{\pi(\theta') q(\theta', \theta)}{\pi(\theta) q(\theta, \theta')}\right) q(\theta, \theta') \\ &= \min(\pi(\theta) q(\theta, \theta'), \pi(\theta') q(\theta', \theta)) \\ &= \pi(\theta') \min\left(1, \frac{\pi(\theta) q(\theta, \theta')}{\pi(\theta') q(\theta', \theta)}\right) q(\theta', \theta) \\ &= \pi(\theta') \alpha(\theta', \theta) q(\theta', \theta). \end{aligned}$$

- We have obviously

$$\begin{aligned} & \left(1 - \int \alpha(\theta, u) q(\theta, u) du \right) \delta_{\theta}(\theta') \pi(\theta) \\ = & \left(1 - \int \alpha(\theta', u) q(\theta', u) du \right) \delta_{\theta'}(\theta) \pi(\theta'). \end{aligned}$$

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- It follows that

$$\pi(\theta) K(\theta, \theta') = \pi(\theta') K(\theta', \theta).$$

- Hence, π is the invariant distribution of the transition kernel K .

- To ensure irreducibility, a sufficient but not necessary condition is that

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Irreducibility and Aperiodicity

- To ensure irreducibility, a sufficient but not necessary condition is that

$$\pi(\theta') > 0 \Rightarrow q(\theta, \theta') > 0.$$

- Aperiodicity is automatically ensured as there is always a strictly positive probability to reject the candidate.
- Theoretically, the MH algorithm converges under very weak assumptions to the target distribution π . In practice, this convergence can be so slow that the algorithm is useless.

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to obtain good performance.

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- In practice, similarly to Rejection sampling or Importance Sampling, you need to ensure that

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to obtain good performance.

- If you don't ensure this condition, the algorithm might give you the impression it works well... but it does NOT.

Examples

- **Example:** Consider the case where

$$\pi(\theta) \propto \exp\left(-\frac{\theta^2}{2}\right).$$

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- We implement the MH algorithm for

$$q_1(\theta) \propto \exp\left(-\frac{\theta^2}{2(0.2)^2}\right)$$

so $\pi(\theta) / q_1(\theta) \rightarrow \infty$ as $\theta \rightarrow \infty$ and for

$$q_2(\theta) \propto \exp\left(-\frac{\theta^2}{2(5)^2}\right)$$

so $\pi(\theta) / q_2(\theta) \leq C < \infty$ for all θ .

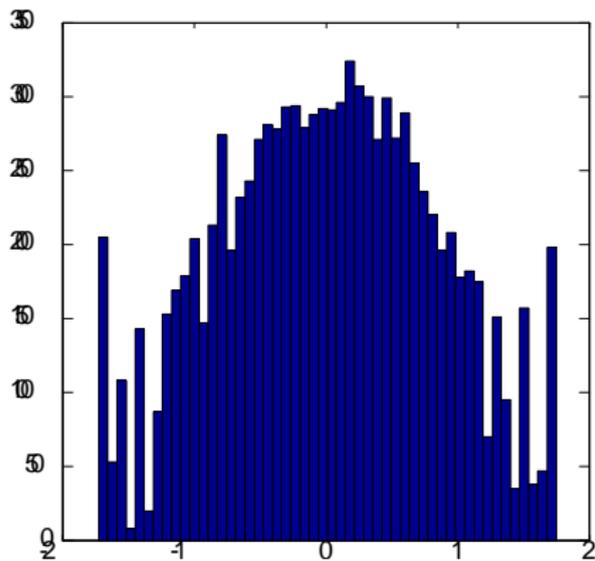
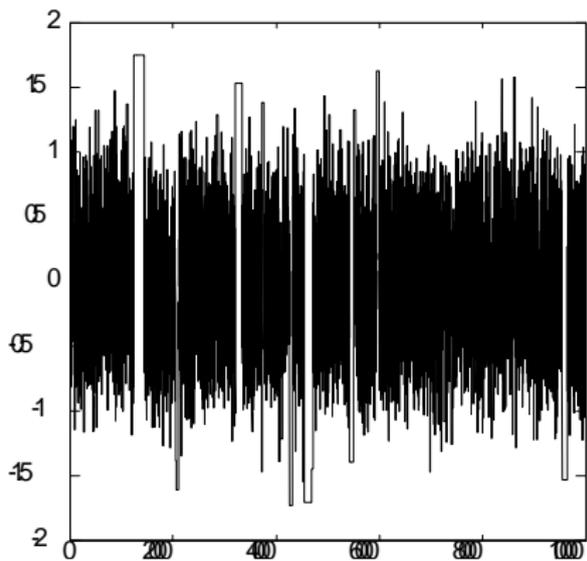


Figure: MCMC output for q_1 , we estimate $\mathbb{E}(\theta) = 0.0206$ and $\mathbb{V}(\theta) = 0.83$.

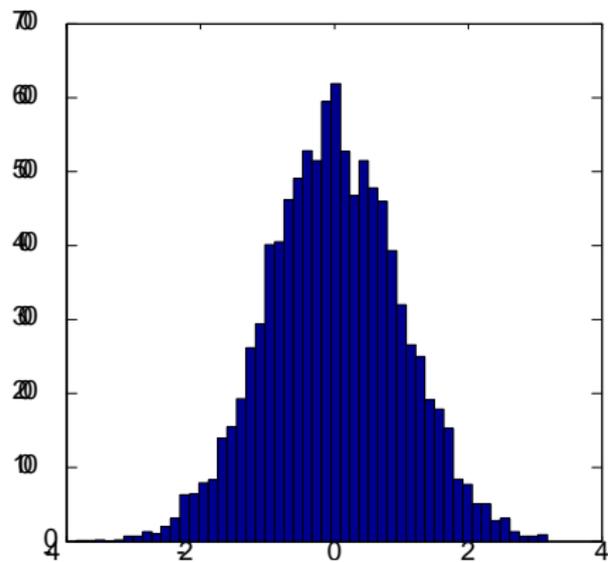
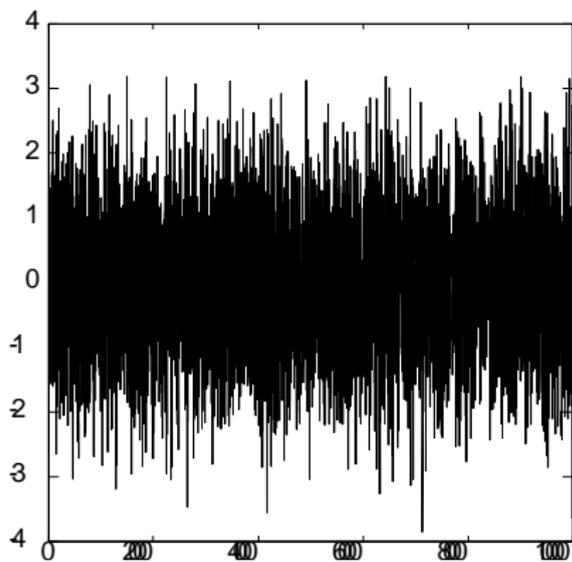


Figure: MCMC output for q_2 , we estimate $\mathbb{E}(\theta) = -0.004$ and $\mathbb{V}(\theta) = 1.00$.

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- When the variance of the random walk increments (if it exists) is very small then the acceptance rate can be expected to be around 0.5-0.7.
- You would like to scale the random walk moves such that it is possible to move reasonably fast in regions of positive probability masses under π .

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- We implement the MH algorithm for

$$q_1(\theta, \theta') \propto \exp\left(-\frac{(\theta' - \theta)^2}{2(0.2)^2}\right),$$

$$q_2(\theta, \theta') \propto \exp\left(-\frac{(\theta' - \theta)^2}{2(5)^2}\right),$$

$$q_3(\theta, \theta') \propto \exp\left(-\frac{(\theta' - \theta)^2}{2(0.02)^2}\right).$$

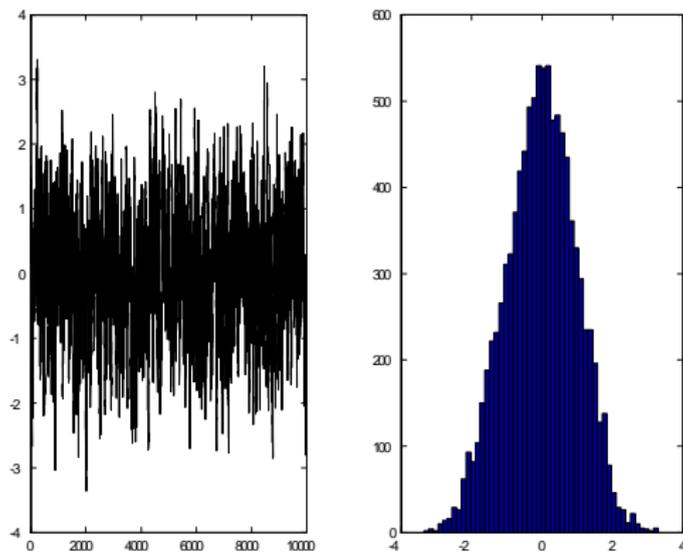


Figure: MCMC output for q_1 , we estimate $\mathbb{E}(\theta) = -0.02$ and $\mathbb{V}(\theta) = 0.99$

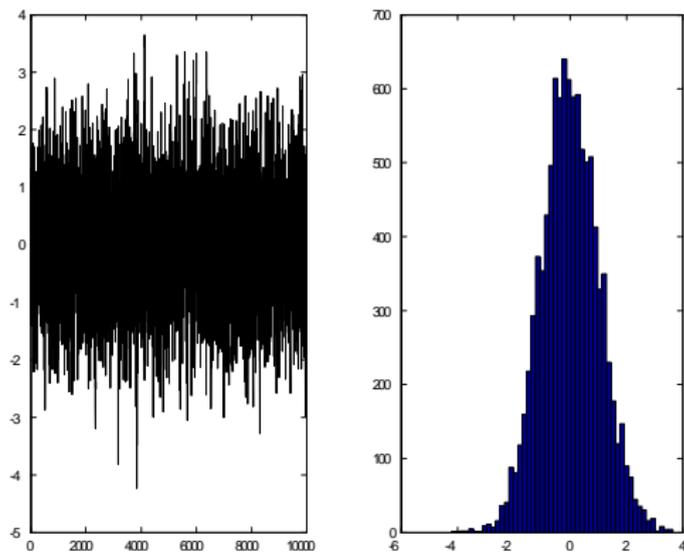


Figure: MCMC output for q_2 , we estimate $\mathbb{E}(\theta) = 0.00$ and $\mathbb{V}(\theta) = 1.02$.

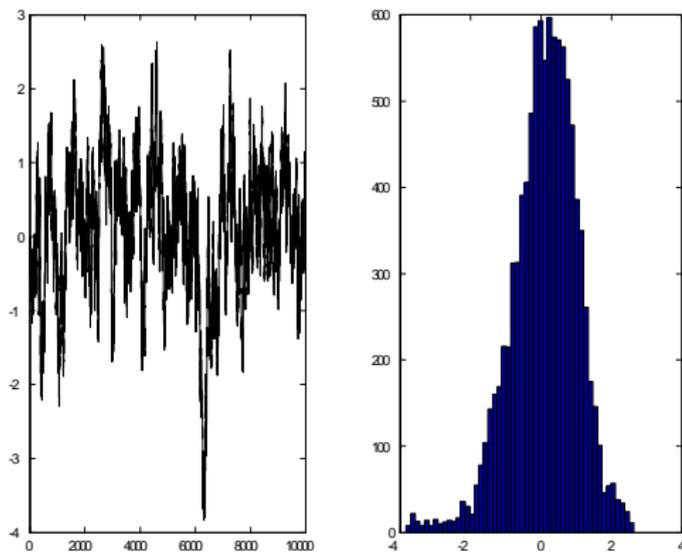


Figure: MCMC output for q_3 , we estimate $\mathbb{E}(\theta) = 0.10$ and $\mathbb{V}(\theta) = 0.92$.

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- It is tempting to adapt the variance of the increments given the simulation output... Unfortunately this breaks the Markov property and biases results if one is not careful.

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- So a good strategy can be to use a proposal distribution of the form

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where $0 < \lambda < 1$.

- This algorithm is definitely valid as it is just a particular case of the MH algorithm.

Mixture of Kernels

- An alternative achieving the same purpose is to use a transition kernel

$$K(\theta, \theta') = \lambda K_1(\theta, \theta') + (1 - \lambda) K_2(\theta, \theta')$$

where K_1 (resp. K_2) is an MH algorithm of proposal q_1 (resp. q_2).

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- This algorithm is different from using $q(\theta, \theta') = \lambda q_1(\theta') + (1 - \lambda) q_2(\theta, \theta')$. It is computationally cheaper and still valid as

$$\begin{aligned} & \int \pi(\theta) K(\theta, \theta') d\theta \\ &= \lambda \int \pi(\theta) K_1(\theta, \theta') d\theta + (1 - \lambda) \int \pi(\theta) K_2(\theta, \theta') d\theta \\ &= \lambda \pi(\theta') + (1 - \lambda) \pi(\theta') \\ &= \pi(\theta') \end{aligned}$$

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- We can use

$$\theta' = \theta + \frac{\sigma^2}{2} \nabla \log \pi(\theta) + \sigma V \text{ where } V \sim \mathcal{N}(0, 1)$$

where σ^2 is selected such that the acceptance ratio is approximately 0.57.

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- The motivation is that, we know that in continuous-time

$$d\theta_t = \frac{1}{2} \nabla \log \pi(\theta) + \sigma dW_t$$

admits π has an invariant distribution.

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- You do not need to have an explicit form for the mapping φ ! As long as φ is a *deterministic* mapping, then it is fine. For example $\varphi(\theta)$ could be the local maximum of π closest to θ that has been determined using a gradient algorithm.
- To compute the acceptance probability of the candidate θ' , you will need to compute $\varphi(\theta')$ and then you can compute the MH acceptance ratio.

- The standard MH algorithm uses the acceptance probability

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- Example (Baker, 1965):

$$\alpha(\theta, \theta') = \frac{\pi(\theta') q(\theta', \theta)}{\pi(\theta') q(\theta', \theta) + \pi(\theta) q(\theta, \theta')}.$$

- Indeed one can check that

$$K(\theta, \theta') = \alpha(\theta, \theta') q(\theta, \theta') + \left(1 - \int \alpha(\theta, u) q(\theta, u) du\right) \delta_{\theta}(\theta')$$

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- We have

$$\begin{aligned} \pi(\theta) \alpha(\theta, \theta') q(\theta, \theta') &= \pi(\theta) \frac{\delta(\theta, \theta')}{\pi(\theta) q(\theta, \theta')} q(\theta, \theta') \\ &= \delta(\theta, \theta') \\ &= \delta(\theta', \theta) \\ &= \pi(\theta') \alpha(\theta', \theta) q(\theta', \theta). \end{aligned}$$

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$$\begin{aligned} \pi(\theta) \alpha(\theta, \theta') q(\theta, \theta') &= \pi(\theta) \frac{\delta(\theta, \theta')}{\pi(\theta) q(\theta, \theta')} q(\theta, \theta') \\ &= \delta(\theta, \theta') \\ &= \delta(\theta', \theta) \\ &= \pi(\theta') \alpha(\theta', \theta) q(\theta', \theta). \end{aligned}$$

- The MH acceptance is favoured as it increases the acceptance probability.

Limitations of the MH algorithm

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- In practice, the choice of the proposal distribution is absolutely crucial on the performance of the algorithm.
- In high dimensional problems, a simple MH algorithm will be useless. It will be necessary to use a combination of MH kernels.... However for the time being you might not have realized the power of the mixture and composition of kernels.

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- We then combine these kernels through mixture or composition.

- The proposal $\bar{q}_1(\theta, \theta')$ associated to $K_1(\theta, \theta')$ is given by

$$\bar{q}_1(\theta, \theta') = \bar{q}_1((\theta_1, \theta_2), (\theta'_1, \theta'_2)) = q_1((\theta_1, \theta_2), \theta'_1) \delta_{\theta_2}(\theta'_2).$$

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- Sample $\theta_1^* \sim q_1 \left(\left(\theta_1^{(i-1)}, \theta_2^{(i-1)} \right), \cdot \right)$ and compute

$$\alpha_1 \left(\left(\theta_1^{(i-1)}, \theta_2^{(i-1)} \right), \left(\theta_1^*, \theta_2^{(i-1)} \right) \right) \\ = \min \left(1, \frac{\pi \left(\theta_1^* \mid \theta_2^{(i-1)} \right) q_1 \left(\left(\theta_1^*, \theta_2^{(i-1)} \right), \theta_1^{(i-1)} \right)}{\pi \left(\theta_1^{(i-1)} \mid \theta_2^{(i-1)} \right) q_1 \left(\left(\theta_1^{(i-1)}, \theta_2^{(i-1)} \right), \theta_1^* \right)} \right)$$

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- With probability $\alpha_1 \left(\left(\theta_1^{(i-1)}, \theta_2^{(i-1)} \right), \left(\theta_1^*, \theta_2^{(i-1)} \right) \right)$, set $\theta_1^{(i)} = \theta_1^*$ and otherwise $\theta_1^{(i)} = \theta_1^{(i-1)}$.

MH step to update component 2

- Sample $\theta_2^* \sim q_2 \left(\left(\theta_1^{(i)}, \theta_2^{(i-1)} \right), \cdot \right)$ and compute

$$\begin{aligned} & \alpha_2 \left(\left(\theta_1^{(i)}, \theta_2^{(i-1)} \right), \left(\theta_1^{(i)}, \theta_2^* \right) \right) \\ = & \min \left(1, \frac{\pi \left(\theta_2^* | \theta_1^{(i)} \right) q_2 \left(\left(\theta_1^{(i)}, \theta_2^* \right), \theta_2^{(i-1)} \right)}{\pi \left(\theta_2^{(i-1)} | \theta_1^{(i)} \right) q_2 \left(\left(\theta_1^{(i)}, \theta_2^{(i-1)} \right), \theta_2^* \right)} \right) \end{aligned}$$

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- With probability $\alpha_2 \left(\left(\theta_1^{(i)}, \theta_2^{(i-1)} \right), \left(\theta_1^{(i)}, \theta_2^* \right) \right)$, set $\theta_2^{(i)} = \theta_2^*$ otherwise $\theta_2^{(i)} = \theta_2^{(i-1)}$.

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- Sample $\theta_J^* \sim q_J\left(\left(\theta_1^{(i-1)}, \theta_2^{(i-1)}\right), \cdot\right)$ and compute

$$\alpha_J\left(\left(\theta_1^{(i-1)}, \theta_2^{(i-1)}\right), \left(\theta_J^*, \theta_{-J}^{(i)}\right)\right) \\ = \min\left(1, \frac{\pi\left(\theta_J^* \mid \theta_{-J}^{(i)}\right) q_J\left(\left(\theta_J^*, \theta_{-J}^{(i)}\right), \theta_J^{(i-1)}\right)}{\pi\left(\theta_J^{(i-1)} \mid \theta_{-J}^{(i)}\right) q_K\left(\left(\theta_J^{(i-1)}, \theta_{-J}^{(i)}\right), \theta_J^*\right)}\right).$$

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- However, the composition and mixture of these kernels can be irreducible and aperiodic because then all the components are updated.

- Consider now the case where

$$q_1((\theta_1, \theta_2), \theta'_1) = \pi(\theta'_1 | \theta_2).$$

then

$$r_1(\theta, \theta') = \frac{\pi(\theta'_1 | \theta_2) q_1((\theta'_1, \theta_2), \theta_1)}{\pi(\theta_1 | \theta_2) q_1((\theta_1, \theta_2), \theta'_1)} = \frac{\pi(\theta'_1 | \theta_2) \pi(\theta_1 | \theta_2)}{\pi(\theta_1 | \theta_2) \pi(\theta'_1 | \theta_2)} = 1$$

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- If you take for proposal distributions in the MH kernels the full conditional distributions then you have the Gibbs sampler!

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- Iteration i ; $i \geq 1$:
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 - Sample $\theta_k^{(i)}$ using an MH step of proposal distribution $q_k\left(\left(\theta_{-k}^{(i)}, \theta_k^{(i-1)}\right), \theta_k'\right)$ and target $\pi\left(\theta_k \mid \theta_{-k}^{(i)}\right)$ where $\theta_{-k}^{(i)} = \left(\theta_1^{(i)}, \dots, \theta_{k-1}^{(i)}, \theta_{k+1}^{(i-1)}, \dots, \theta_p^{(i-1)}\right)$.

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- **Example:** Assume we have $\pi(\theta_1, \theta_2)$ where it is easy to sample from $\pi(\theta_1 | \theta_2)$ and then use an MH step of invariant distribution $\pi(\theta_2 | \theta_1)$.

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- Sample $\theta_1^{(i)} \sim \pi(\theta_1 | \theta_2^{(i-1)})$.
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- There is **NO NEED** to run the MH algorithm multiple steps to ensure that $\theta_2^{(i)} \sim \pi(\theta_2 | \theta_2^{(i-1)})$.

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- You are now equipped to fit advanced statistical models...