Modern Computational Statistics

Lecture 6&7: Markov Chain Monte Carlo

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October 07, 2019

Limitations of Monte Carlo

- Direct sampling in high-dimensional spaces is often infeasible, very hard to get rare events
- Rejection sampling, Importance sampling
  - Do not work well if the proposal $q(x)$ is very different from $f(x)$ or $h(x)f(x)$.
  - Moreover, constructing appropriate $q(x)$ can be difficult. Making a good proposal usually requires knowledge of the analytic form of the target distribution - but if we had that, we wouldn't even need to sample
- Intuition: instead of a fixed proposal $q(x)$, what if we use an adaptive proposal?
- In this lecture, we are going to talk about one of the most popular sampling methods, **Markov chain Monte Carlo**.

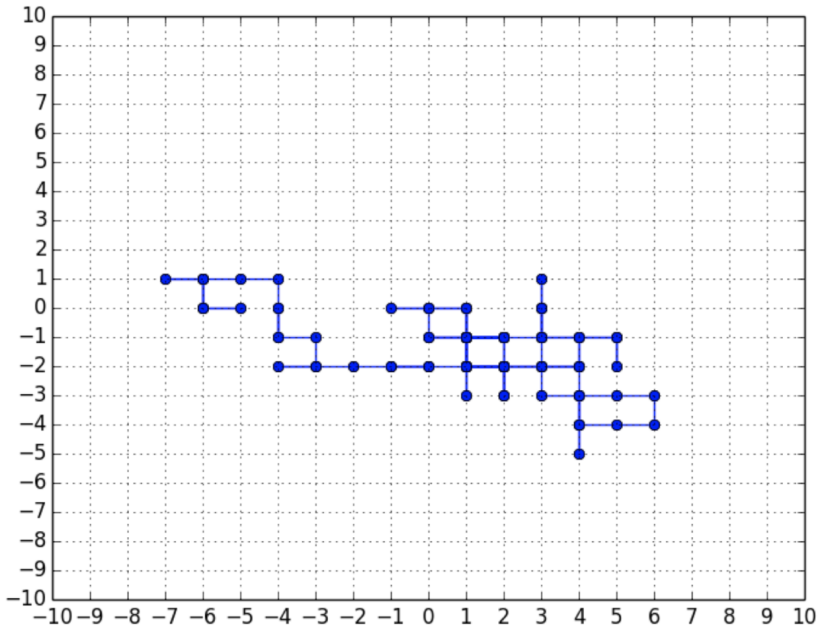
- Stochastic processes is a family of random variables, usually indexed by a set of numbers (time). A discrete time stochastic process is simply a sequence of random variables, $X_0, X_1, \ldots, X_n$ defined on the same probability space
- One of the simplest stochastic processes (and one of the most useful) is the simple random walk
- Consider a simple random walk on a graph $G = (\Omega, E)$. The stochastic process starts from an initial position $X_0 = x_0 \in \Omega$, and proceeds following a simple rule:

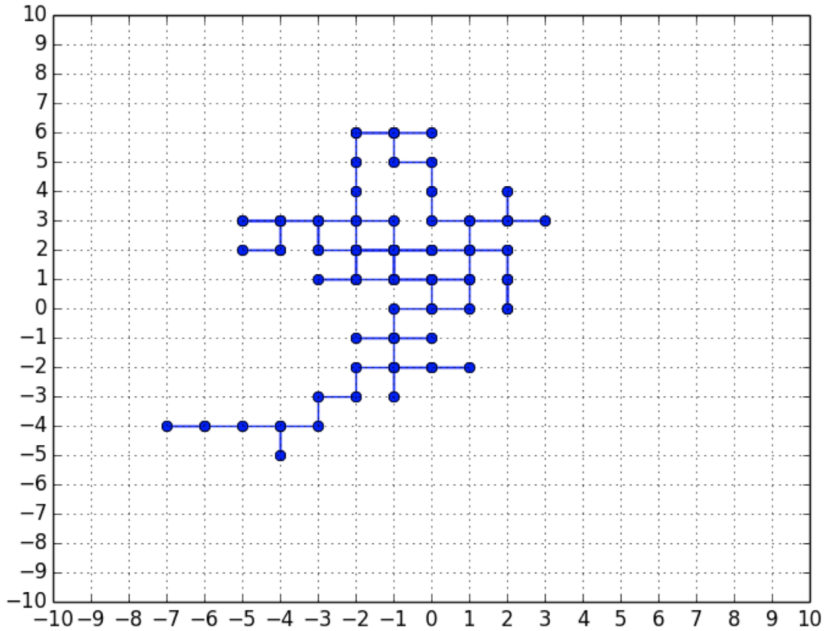
$$p(X_{n+1}|X_n = x_n) \sim \text{Discrete}(\mathcal{N}(x_n)),\ \forall n \geq 0$$

where $\mathcal{N}(x_n)$ denotes the neighborhood of x_n

Example

Two random walks on a 10×10 grid graph





- The above simple random walk is a special case of another well-known stochastic process called *Markov chains*
- A Markov chain represents the stochastic movement of some particle in the state space over time. The particle initially starts from state i with probability $\pi_i^{(0)}$, and after that moves from the current state i at time t to the next state j with probability $p_{ij}(t)$
- A Markov chain has three main elements:
  1. A state space $\mathcal{S}$
  2. An initial distribution $\pi^{(0)}$ over $\mathcal{S}$
  3. Transition probabilities $p_{ij}(t)$ which are non-negative numbers representing the probability of going from state i to j, and $\sum_j p_{ij}(t) = 1$.
- When $p_{ij}(t)$ does not depend on time t, we say the Markov chain is time-homegenous

- Chain rule (in probability)

$$p(X_n = x_n, \ldots, X_0 = x_0) = \prod_{i=1}^{n} p(X_i = x_i | X_{<i} = x_{<i})$$

- **Markov property**

$$p(X_{i+1} = x_{i+1} | X_i = x_i, \ldots, X_0 = x_0) = p(X_{i+1} = x_{i+1} | X_i = x_i)$$

- Joint probability with Markov property

$$p(X_n = x_n, \ldots, X_0 = x_0) = \prod_{i=1}^{n} p(X_i = x_i | X_{i-1} = x_{i-1})$$

fully determined by the transition probabilities

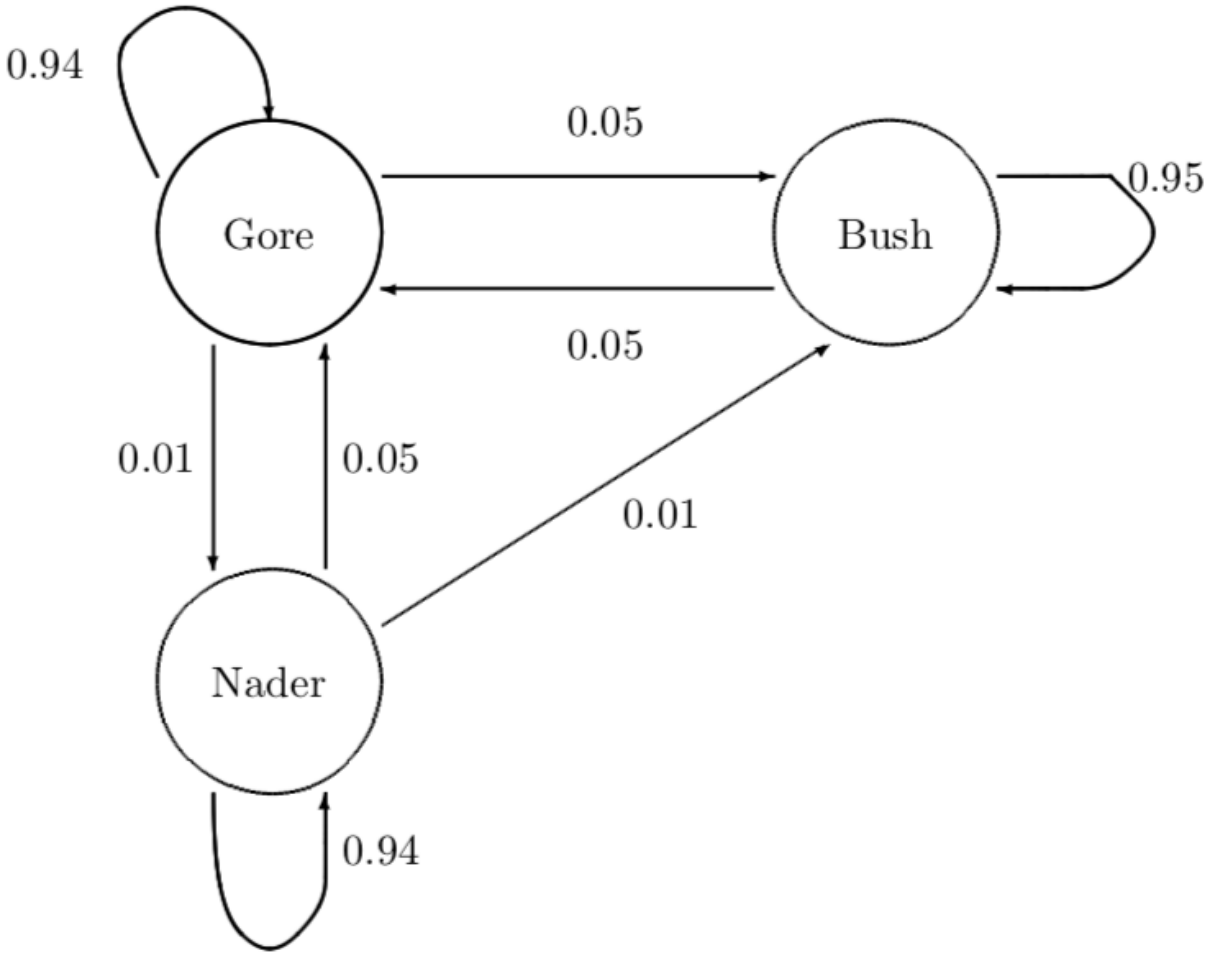
Example

- Consider the 2000 US presidential election with three candidates: Gore, Bush and Nader (just an illustrative example and does not reflect the reality of that election)
- We assume that the initial distribution of votes (i.e., probability of winning) was $\pi = (0.49, 0.45, 0.06)$ for Gore, Bush and Nader respectively
- Further, we assume the following transition probability matrix

	Gore	*Bush*	*Nader*
Gore	0.94	0.05	0.01
Bush	0.05	0.95	0
Nader	0.05	0.01	0.94

Example

A probabilistic graph presentation of the Markov chain



- If we represent the transition probability a square matrix P such that $P_{ij} = p_{ij}$, we can obtain the distribution of states in step n, $\pi^{(n)}$, as follows

$$\pi^{(n)} = \pi^{(n-1)} P = \ldots = \pi^{(0)} P^n$$

- For the above example, we have

$$\begin{aligned}
\pi^{(0)} &= (0.4900, 0.4500, 0.0600) \\
\pi^{(10)} &= (0.4656, 0.4655, 0.0689) \\
\pi^{(100)} &= (0.4545, 0.4697, 0.0758) \\
\pi^{(200)} &= (0.4545, 0.4697, 0.0758)
\end{aligned}$$

- As we can see last, after several iterations, the above Markov chain converges to a distribution, $(0.4545, 0.4697, 0.0758)$
- In this example, the chain would have reached this distribution regardless of what initial distribution $\pi^{(0)}$ we chose. Therefore, $\pi = (0.4545, 0.4697, 0.0758)$ is the stationary distribution for the above Markov chain
- **Stationary distribution**. A distribution of Markov chain states is called to be stationary if it remains the same in the next time step, i.e.,

$$\pi = \pi P$$

- How can we find out whether such distribution exists?
- Even if such distribution exists, is it unique or not?
- Also, how do we know whether the chain would converge to this distribution?
- To find out the answer, we briefly discuss some properties of Markov chains

Irreducibility

- Irreducible: A Markov chain is irreducible if the chain can move from any state to another state.
- Examples
  - The simple random walk is irreducible
  - The following chain, however, is reducible since Nader does not communicate with the other two states (Gore and Bush)

	Gore	*Bush*	*Nader*
Gore	0.95	0.05	0
Bush	0.05	0.95	0
Nader	0	0	1

Aperiodicity

- Period: the period of a state i is the greatest common divisor of the times at which it is possible to move from i to i.
- For example, all the states in the following Markov chain have period 3.

$$\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}$$

- Aperiodic: a Markov chain is said to be aperiodic if the period of each state is 1, otherwise the chain is periodic.

- **Recurrent** states: a state i is called recurrent if with probability 1, the chain would ever return to state i given that it started in state i.

	Gore	*Bush*	*Nader*
Gore	0.94	0.05	0.01
Bush	0.05	0.95	0
Nader	0.05	0.01	0.94

- **Positive recurrent**: a recurrent state j is called positive recurrent if the expected amount of time to return to state j given that the chain started in state j is finite
- For a positive recurrent Markov chain, the stationary distribution exists and is unique

- **Reversibility**: a Markov chain is said to be reversible with respect to a probability distribution π if $\pi_i p_{ij} = \pi_j p_{ji}$
- In fact, if a Markov chain is reversible with respect to π, then π is also a stationary distribution

$$\begin{aligned}\sum_i \pi_i p_{ij} &= \sum_i \pi_j p_{ji} \\ &= \pi_j \sum_i p_{ji} \\ &= \pi_j\end{aligned}$$

since $\sum_i p_{ij} = 1$ for all transition probability matrices

- This is also known as *detailed balance condition*

- We can define a Markov chain on a general state space $\mathcal{X}$ with initial distribution $\pi^{(0)}$ and transition probabilities $p(x, A)$ defined as the probability of jumping to the subset A from point $x \in \mathcal{X}$
- Similarly, with Markov property, we have the joint probability

$$p(X_0 \in A_0, \ldots, X_n \in A_n) = \int_{A_0} \pi^{(0)}(dx_0) \ldots \int_{A_n} p(x_{n-1}, dx_n)$$

- Example. Consider a Markov chain with the real line as its state space. The initial distribution is $\mathcal{N}(0, 1)$, and the transition probability is $p(x, \cdot) = \mathcal{N}(x, 1)$. This is just a Brownian motion (observed at discrete time)

ϕ-irreducibility and ϕ-aperiodicity

- Unlike the discrete space, we now need to talk about the property of Markov chains with a continuous non-zero measure ϕ, on $\mathcal{X}$, and use sets A instead of points
- A chain is ϕ-irreducible if for all $A \subseteq \mathcal{X}$ with $\phi(A) > 0$ and for all $x \in \mathcal{X}$, there exists a positive integer n such that

$$p^n(x, A) = p(X_n \in A | X_0 = x) > 0$$

- Similarly, we need to modify our definition of period

- A distribution π is a stationary distribution if

$$\pi(A) = \int_A \pi(dx)p(x, A), \quad \forall A \subseteq \mathcal{X}$$

- As for the discrete case, a continuous space Markov chain is reversible with respect to π if

$$\pi(dx)p(x, dy) = \pi(dy)p(y, dx)$$

- Similarly, if the chain is reversible with respect to π, then π is a stationary distribution
- Example. Consider a Markov chain on the real line with initial distribution $\mathcal{N}(1, 1)$ and transition probability $p(x, \cdot) = \mathcal{N}(\frac{x}{2}, \frac{3}{4})$. It is easy to show that the chain converges to $\mathcal{N}(0, 1)$ (Exercise)

- Ergodic: a Markov chain is ergodic if it is both irreducible and aperiodic, with stationary distribution π
- **Ergodic Theorem**. For an ergodic Markov chain on the state space $\mathcal{X}$ having stationary distribution π, we have: (i) for all measurable $A \subseteq \mathcal{X}$ and π-a.e. $x \in \mathcal{X}$,

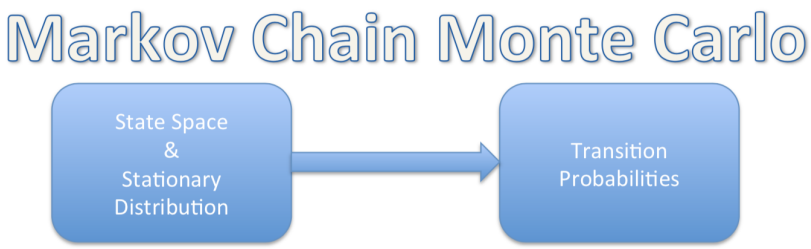
$$\lim_{t\to\infty} p^n(x, A) = \pi(A)$$

(ii) $\forall f$ with $\mathbb{E}_\pi|f(x)| < \infty$,

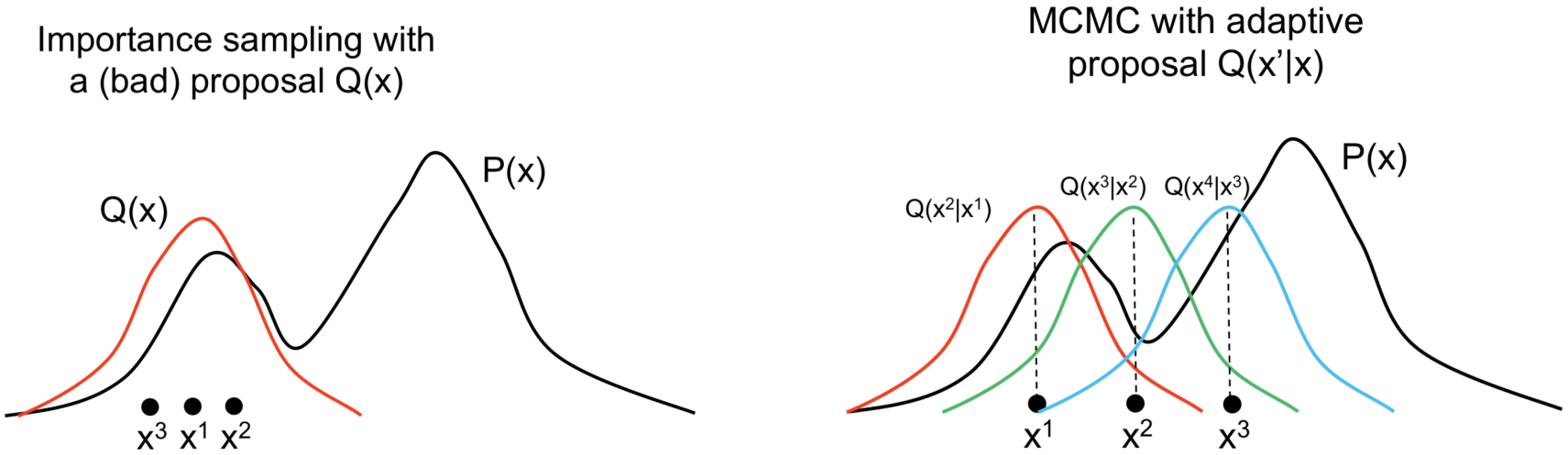
$$\lim_{T\to\infty} \frac{1}{T}\sum_{t=1}^{T} f(X_t) = \int_{\mathcal{X}} f(x)\pi(x)dx, \quad \text{a.s.}$$

In particular, π is the unique stationary probability density function for the chain

- Now suppose we are interested in sampling from a distribution π (e.g., with density $P(x)$, if it is continuous)
- Markov chain Monte Carlo (MCMC) is a method that samples from a Markov chain whose stationary distribution is the target distribution π. It does this by constructing an appropriate transition probability for π
- MCMC, therefore, can be viewed as an inverse process of Markov chains



- The transition probability in MCMC resembles the proposal distribution we used in previous Monte Carlo methods.
- Instead of using a fixed proposal (as in importance sampling and rejection sampling), MCMC algorithms feature adaptive proposals



Figures adapted from Eric Xing (CMU)

- Suppose that we are interested in sampling from a distribution π, whose density we know up to a constant $P(x) \propto \pi(x)$
- We can construct a Markov chain with a transition probability (i.e., proposal distribution) $Q(x'|x)$ which is symmetric; that is, $Q(x'|x) = Q(x|x')$
- Example. A normal distribution with the mean at the current state and fixed variance σ^2 is symmetric since

$$\exp\left(-\frac{(y-x)^2}{2\sigma^2}\right) = \exp\left(-\frac{(x-y)^2}{2\sigma^2}\right)$$

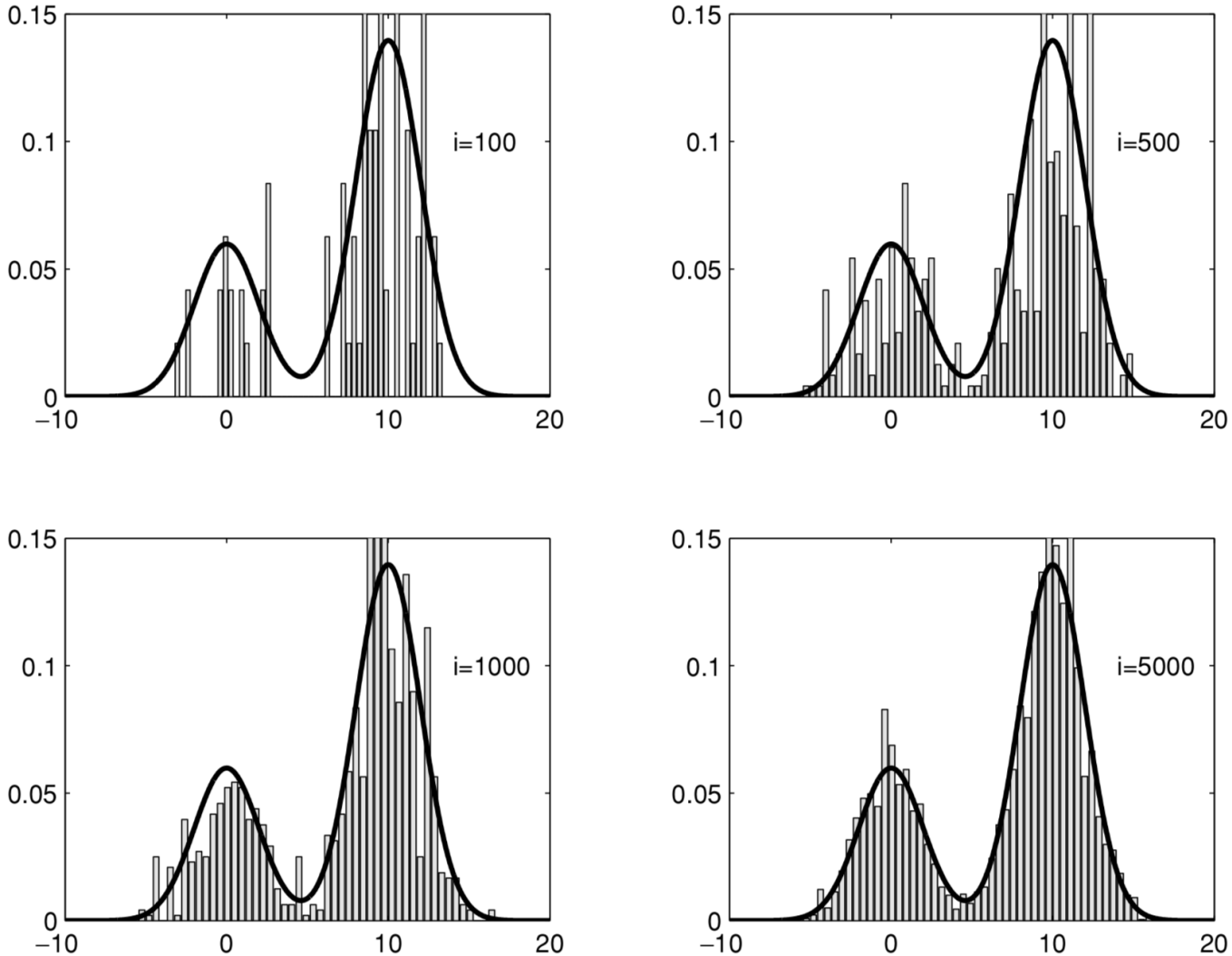
In each iteration we do the following

- Draws a sample x' from $Q(x'|x)$, where x is the previous sample
- Calculated the acceptance probability

$$a(x'|x) = \min\left(1, \frac{P(x')}{P(x)}\right)$$

  Note that we only need to compute $\frac{P(x')}{P(x)}$, the unknown constant cancels out
- Accept the new sample with probability $a(x'|x)$ or remain at state x. The acceptance probability ensures that, after sufficient many draws, our samples will come from the true distribution $\pi(x)$

Example: Gaussian Mixture Model



Adapted from Andrieu, Freitas, Doucet, Jordan, 2003

- How do we know that the chain is going to converge to π?
- Suppose the support of the proposal distribution is $\mathcal{X}$ (e.g., Gaussian distribution), then the Markov chain is irreducible and aperiodic.
- We only need to verify the detailed balance condition

$$\begin{aligned}
\pi(dx)p(x,dx') &= \pi(x)dx \cdot Q(x'|x)a(x'|x)dx' \\
&= \pi(x)Q(x'|x)\min\left(1, \frac{\pi(x')}{\pi(x)}\right)dxdx' \\
&= Q(x'|x)\min(\pi(x), \pi(x'))dxdx' \\
&= Q(x|x')\min(\pi(x'), \pi(x))dxdx' \\
&= \pi(x')dx' \cdot Q(x|x')\min\left(1, \frac{\pi(x)}{\pi(x')}\right)dx \\
&= \pi(dx')p(x',dx)
\end{aligned}$$

- It turned out that symmetric proposal distribution is not necessary. Hastings (1970) later on generalized the above algorithm using the following acceptance probability for general $Q(x'|x)$

$$a(x'|x) = \min\left(1, \frac{P(x')Q(x|x')}{P(x)Q(x'|x)}\right)$$

- Similarly, we can show that detailed balanced condition is preserved

Proposal Distribution

- Under mild assumptions on the proposal distribution Q, the algorithm is ergodic
- However, the choice of Q is important since it determines the speed of convergence to π and the efficiency of sampling
- Usually, the proposal distribution depend on the current state. But it can be independent of current state, which leads to an independent MCMC sampler that is somewhat like a rejection/importance sampling method
- Some examples of commonly used proposal distributions
  - $Q(x'|x) \sim \mathcal{N}(x, \sigma^2)$
  - $Q(x'|x) \sim \text{Uniform}(x - \delta, x + \delta)$
- Finding a good proposal distribution is hard in general

Examples: Gaussian Model with Known Variance

- Recall the univariate Gaussian model with known variance

$$y_i \sim \mathcal{N}(\theta, \sigma^2)$$

$$p(y|\theta, \sigma) = \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi\sigma}} \exp\left(-\frac{(y_i - \theta)^2}{2\sigma^2}\right)$$

- Note that there is a conjugate $\mathcal{N}(\mu_0, \tau_0^2)$ prior for θ, and the posterior has a close form normal distribution
- Now let's pretend that we don't know this exact posterior distribution and use a Markov chain to sample from it.

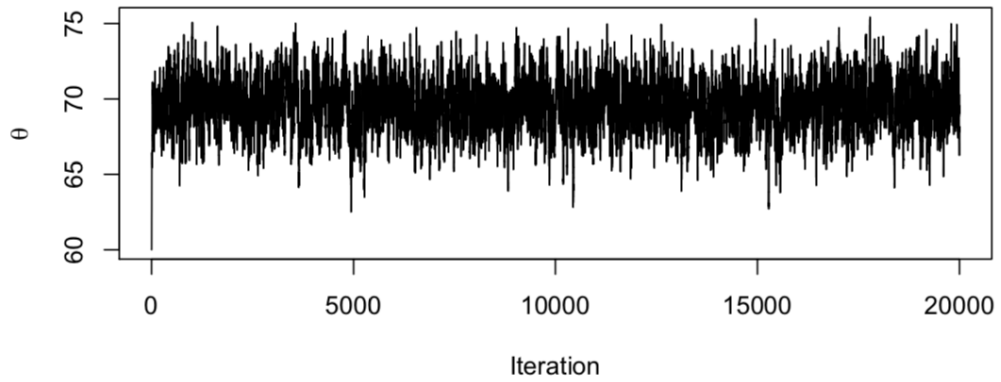
- We can of course write the posterior distribution up to a constant

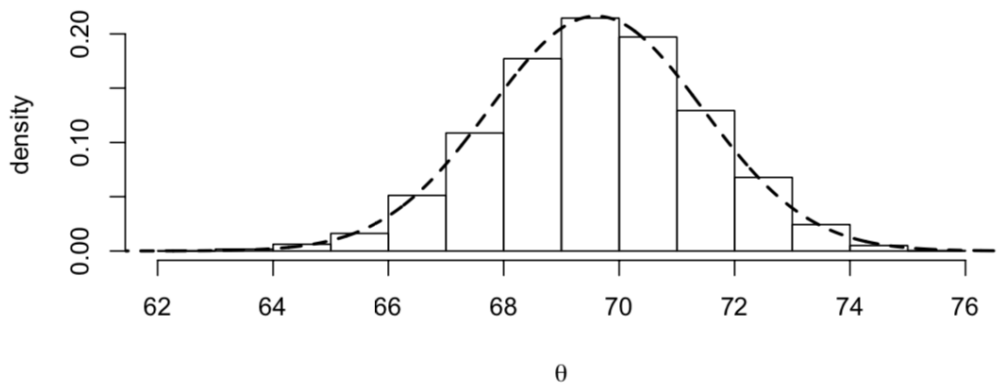
$$p(\theta|y) \propto \exp\left(\frac{(\theta-\mu_0)^2}{2\tau_0^2}\right)\prod_{i=1}^{n}\exp\left(-\frac{(y_i-\theta)^2}{2\sigma^2}\right) = P(\theta)$$

- We use $\mathcal{N}(\theta^{(i)}, 1)$, a normal distribution around our current state, to propose the next step
- Starting from an initial point $\theta^{(0)}$ and propose the next step $\theta' \sim \mathcal{N}(\theta^{(0)}, 1)$, we either accept this value with probability $a(\theta'|\theta^{(0)})$ or reject and stay where we are
- We continue these steps for many iterations

Examples: Gaussian Model with Known Variance

- As we can see, the posterior distribution we obtained using the Metropolis algorithm is very similar to the exact posterior





Example: Poisson Model with Gamma Prior

- Now suppose we want to model the number of half court shots Stephen Curry has made in a game using Poisson model

$$y_i \sim \text{Poisson}(\theta)$$

- He made 0 and 1 half court shots in the first two games respectively
- We used Gamma$(1.4, 10)$ prior for θ, and because of conjugacy, the posterior distribution also had a Gamma distribution

$$\theta|y \sim \text{Gamma}(2.4, 12)$$

- Again, let's ignore the closed form posterior and use MCMC for sampling the posterior distribution

Examples: Poisson Model with Gamma Prior

- The prior is
$$p(\theta) \propto \theta^{0.4} \exp(-10\theta)$$
- The likelihood is
$$p(y|\theta) \propto \theta^{y_1+y_2} \exp(-2\theta)$$
where $y_1 = 0$ and $y_2 = 1$
- Therefore, the posterior is proportional to
$$p(\theta|y) \propto \theta^{0.4} \exp(-10\theta) \cdot \theta^{y_1+y_2} \exp(-2\theta) = P(\theta)$$

- Symmetric proposal distributions such as

$$\text{Uniform}(\theta^{(i)} - \delta, \theta^{(i)} + \delta) \text{ or } \mathcal{N}(\theta^{(i)}, \sigma^2)$$

  might not be efficient since they do not take the non-negative support of the posterior into account.
- Here, we use a non-symmetric proposal distribution such as $\text{Uniform}(0, \theta^{(i)} + \delta)$ and use the Metropolis-Hastings (MH) algorithm instead
- We set $\delta = 1$

We start from $\theta_0 = 1$ and follow these steps in each iteration

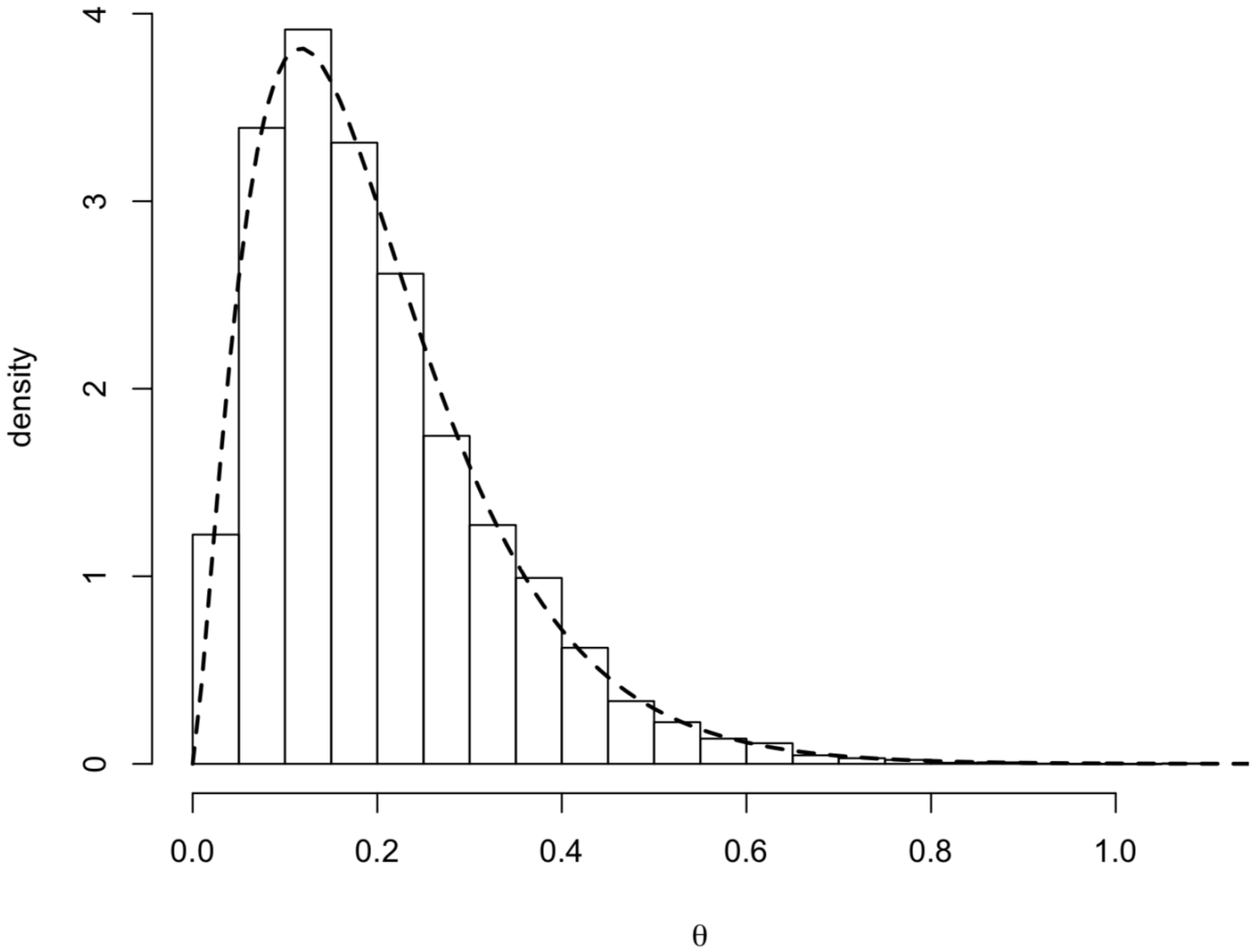
- Sample θ' from $\mathcal{U}(0, \theta^{(i)} + 1)$
- Calculate the acceptance probability

$$a(\theta'|\theta^{(i)}) = \min\left(1, \frac{P(\theta')/(\theta'+1)}{P(\theta^{(i)})/(\theta^{(i)}+1)}\right)$$

- Sample $u \sim \mathcal{U}(0,1)$ and set

$$\theta^{(i+1)} = \begin{cases} \theta' & u < a(\theta'|\theta^{(i)}) \\ \theta^{(i)} & \text{otherwise} \end{cases}$$

Examples: Poisson Model with Gamma Prior



- What if the distribution is multidimensional, *i.e.*, $x = (x_1, x_2, \ldots, x_d)$
- We can still use the Metropolis algorithm (or MH), with a multivariate proposal distribution, *i.e.*, we now propose $x' = (x'_1, x'_2, \ldots, x'_d)$
- For example, we can use a multivariate normal $\mathcal{N}_d(x, \sigma^2 I)$, or a d-dimensional uniform distribution around the current state

Examples: Banana Shape Distribution

- Here we construct a banana-shaped posterior distribution as follows

$$y|\theta \sim \mathcal{N}(\theta_1 + \theta_2^2, \sigma_y^2), \quad \sigma_y = 2$$

  We generate data $y_i \sim \mathcal{N}(1, \sigma_y^2)$
- We use a bivariate normal prior for θ

$$\theta = (\theta_1, \theta_2) \sim \mathcal{N}(0, I)$$

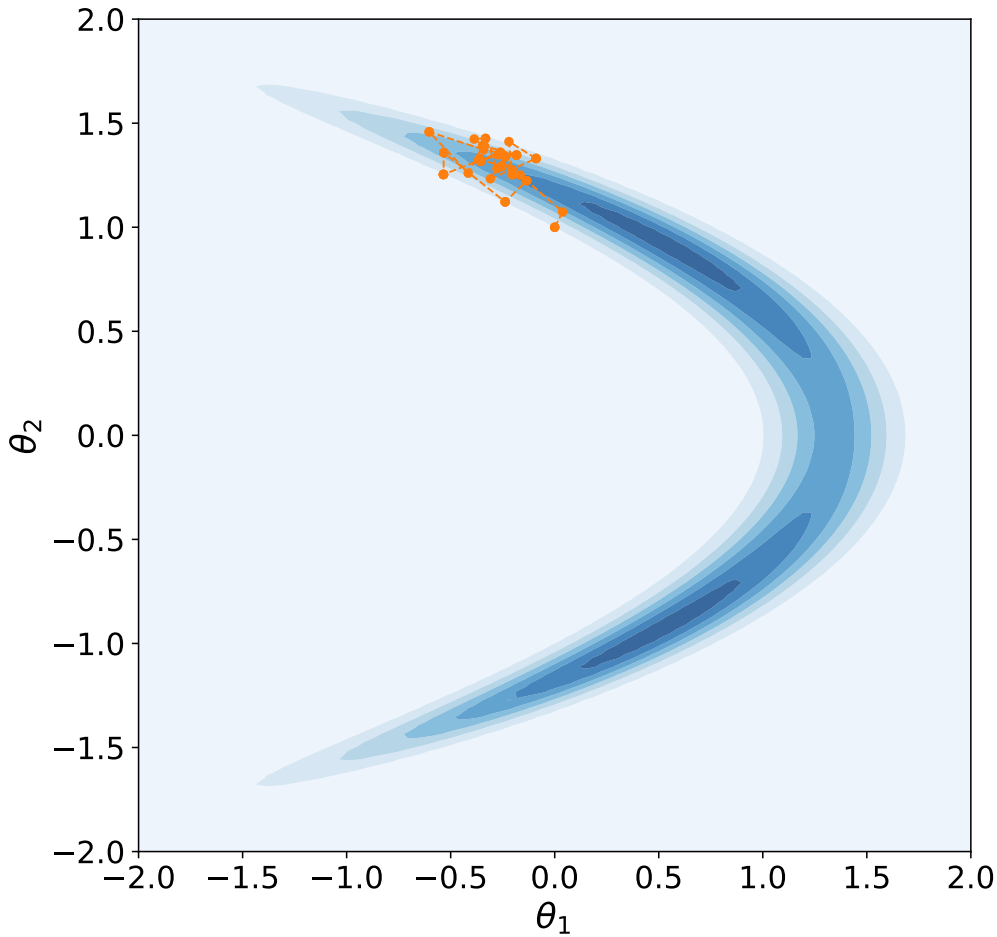
- The posterior is

$$p(\theta|y) \propto \exp\left(-\frac{\theta_1^2 + \theta_2^2}{2}\right) \cdot \exp\left(-\frac{\sum_i (y_i - \theta_1 - \theta_2^2)^2}{2\sigma_y^2}\right)$$

- We use the Metropolis algorithm to sample from posterior, with a bivariate normal proposal distribution such as $\mathcal{N}(\theta^{(i)}, (0.15)^2 I)$

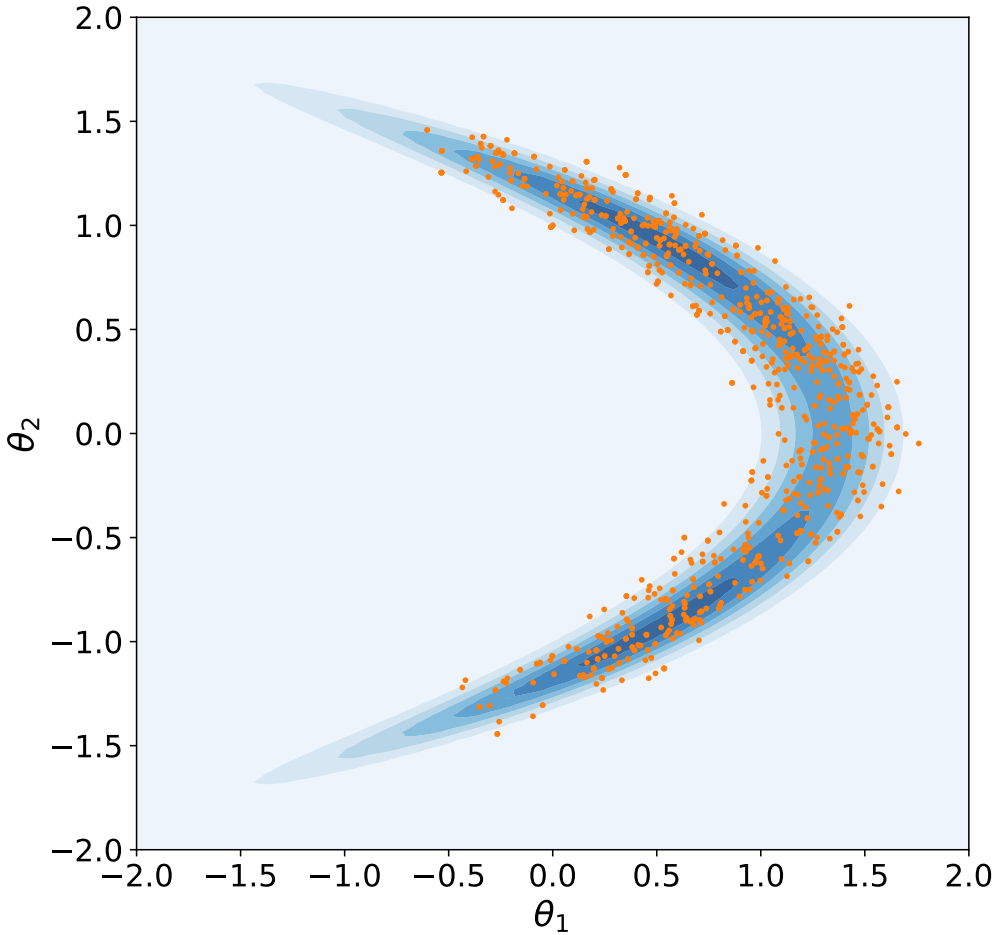
Examples: Banana Shape Distribution

The first few samples from the posterior distribution of $\theta = (\theta_1, \theta_2)$, using a bivariate normal proposal



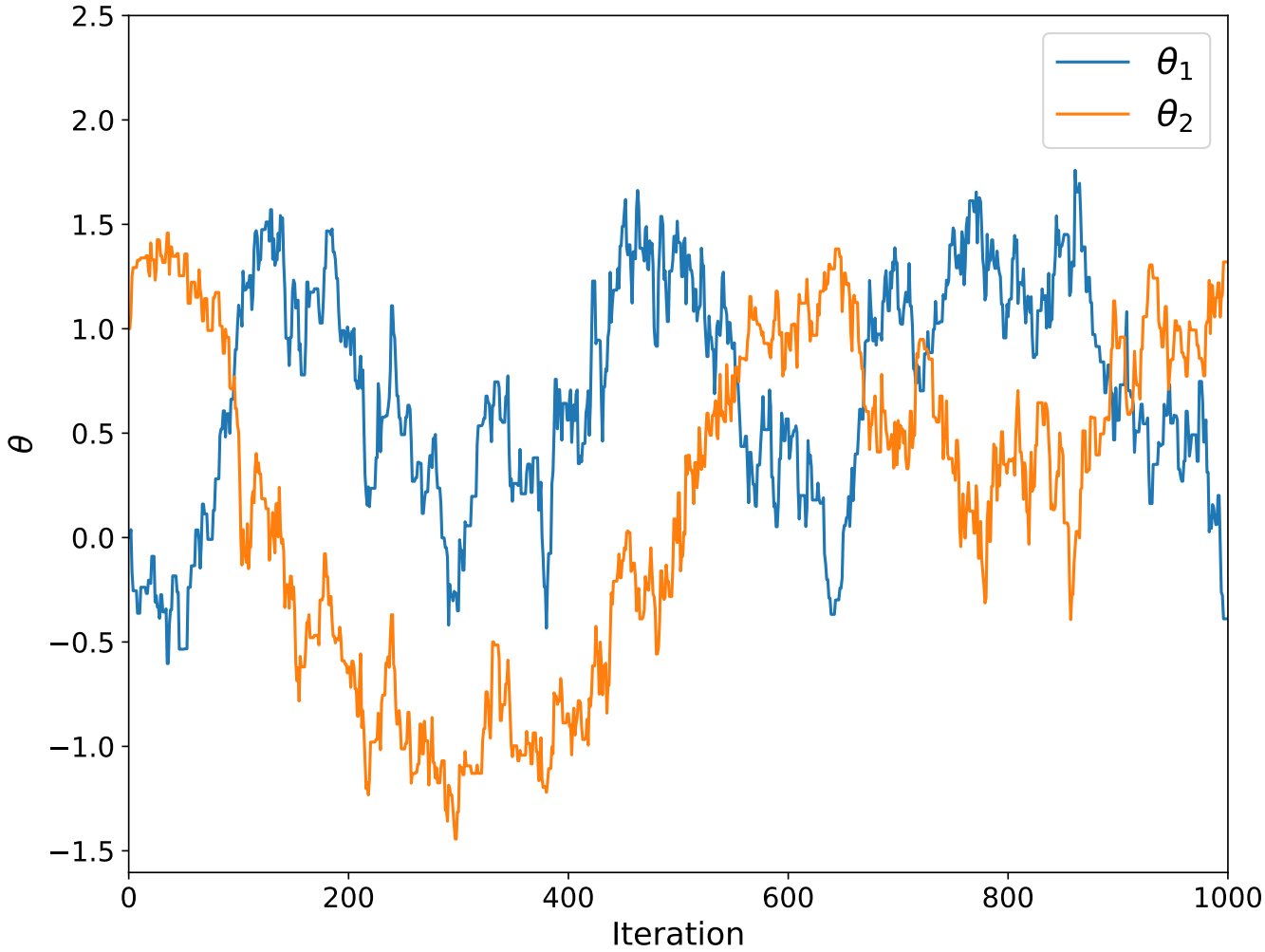
Examples: Banana Shape Distribution

Posterior samples for $\theta = (\theta_1, \theta_2)$



Examples: Banana Shape Distribution

Trace plot of posterior samples for $\theta = (\theta_1, \theta_2)$



Decomposing the Parameter Space

- Sometimes, it is easier to decompose the parameter space into several components, and use the Metropolis (or MH) algorithm for one component at a time
- At iteration i, given the current state $(x_1^{(i)}, \ldots, x_d^{(i)})$, we do the following for all components $k = 1, 2, \ldots, d$
  - Sample x_k' from the univariate proposal distribution $Q(x_k' | \ldots, x_{k-1}^{(i+1)}, x_k^{(i)}, \ldots)$
  - Accept this new value and set $x_k^{(i+1)} = x_k'$ with probability

$$a(x_k' | \ldots, x_{k-1}^{(i+1)}, x_k^{(i)}, \ldots)) = \min\left(1, \frac{P(\ldots, x_{k-1}^{(i+1)}, x_k', \ldots)}{P(\ldots, x_{k-1}^{(i+1)}, x_k^{(i)}, \ldots)}\right)$$

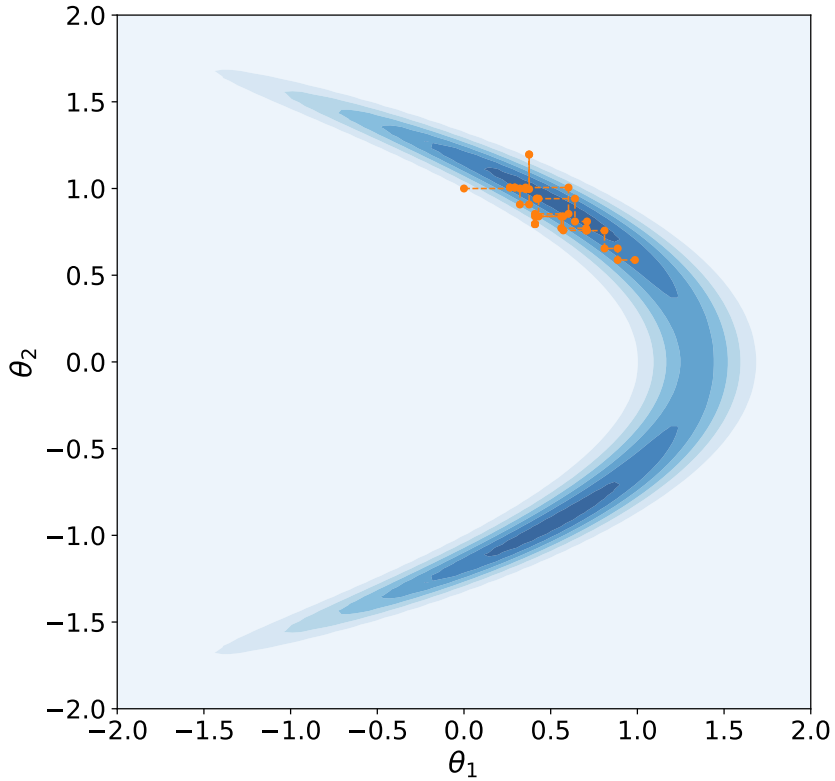
  or reject it and set $x_k^{(i+1)} = x_k^{(i)}$

Decomposing the Parameter Space

- Note that in general, we can decompose the space of random variable into blocks of components
- Also, we can update the components sequentially or randomly
- As long as each transition probability individually leaves the target distribution invariant, their sequence would leave the target distribution invariant
- In Bayesian models, this is especially useful if it is easier and computationally less intensive to evaluate the posterior distribution when one subset of parameters change at a time

Example: Banana Shape Distribution

- In the example of banana-shaped distribution, we can sample θ_1 and θ_2 one at a time
- The first few samples from the posterior distribution of $\theta = (\theta_1, \theta_2)$, using a univariate normal proposal sequentially



- As the dimensionality of the parameter space increases, it becomes difficult to find an appropriate proposal distributions (e.g., with appropriate step size) for the Metropolis (or MH) algorithm
- If we are lucky (in some situations we are!), the conditional distribution of one component, x_j, given all other components, x_{-j} is tractable and has a close form so that we can sample from it directly
- If that's the case, we can sample from each component one at a time using their corresponding conditional distributions $P(x_j|x_{-j})$

- This is known as the Gibbs sampler (GS) or "heat bath" (Geman and Geman, 1984)
- Note that in Bayesian analysis, we are mainly interested in sampling from $p(\theta|y)$
- Therefore, we use the Gibbs sampler when $P(\theta_j|y, \theta_{-j})$ has a closed form, e.g., there is a conditional conjugacy
- One example is the univariate normal model. As we will see later, given σ, the posterior $P(\mu|y, \sigma^2)$ has a closed form, and given μ, the posterior distribution of $P(\sigma^2|\mu, y)$ also has a closed form

The Gibbs Sampler

- The Gibbs sampler works as follows
- Initialize starting value for $x_1, x_2, \ldots, x_d$
- At each iteration, pick an ordering of the d variables (can be sequential or random)
  1. Sample $x \sim P(x_i | x_1, \ldots, x_{i-1}, x_{i+1}, \ldots, x_d)$, *i.e.*, the conditional distribution of x_i given the current values of all other variables
  2. Update $x_i \leftarrow x$
- When we update x_i, we immediately use it new value for sampling other variables x_j

GS is A Special Case of MH

- Note that in GS, we are not proposing anymore, we are directly sampling, which can be viewed as a proposal that will always be accepted
- This way, the Gibbs sampler can be viewed as a special case of MH, whose proposal is

$$Q(x_i', x_{-i}|x_i, x_{-i}) = P(x_i'|x_{-i})$$

- Applying MH with this proposal, we obtain

$$a(x_i', x_{-i}|x_i, x_{-i}) = \min\left(1, \frac{P(x_i', x_{-i})Q(x_i, x_{-i}|x_i', x_{-i})}{P(x_i, x_{-i})Q(x_i', x_{-i}|x_i, x_{-i})}\right)$$

$$= \min\left(1, \frac{P(x_i', x_{-i})P(x_i|x_{-i})}{P(x_i, x_{-i})P(x_i'|x_{-i})}\right) = \min\left(1, \frac{P(x_i', x_{-i})P(x_i, x_{-i})}{P(x_i, x_{-i})P(x_i', x_{-i})}\right)$$

$$= 1$$

- We can now use the Gibbs sampler to simulate samples from the posterior distribution of the parameters of a univariate normal $y \sim \mathcal{N}(\mu, \sigma^2)$ model, with prior

$$\mu \sim \mathcal{N}(\mu_0, \tau_0^2), \quad \sigma^2 \sim \text{Inv-}\chi^2(\nu_0, \sigma_0^2)$$

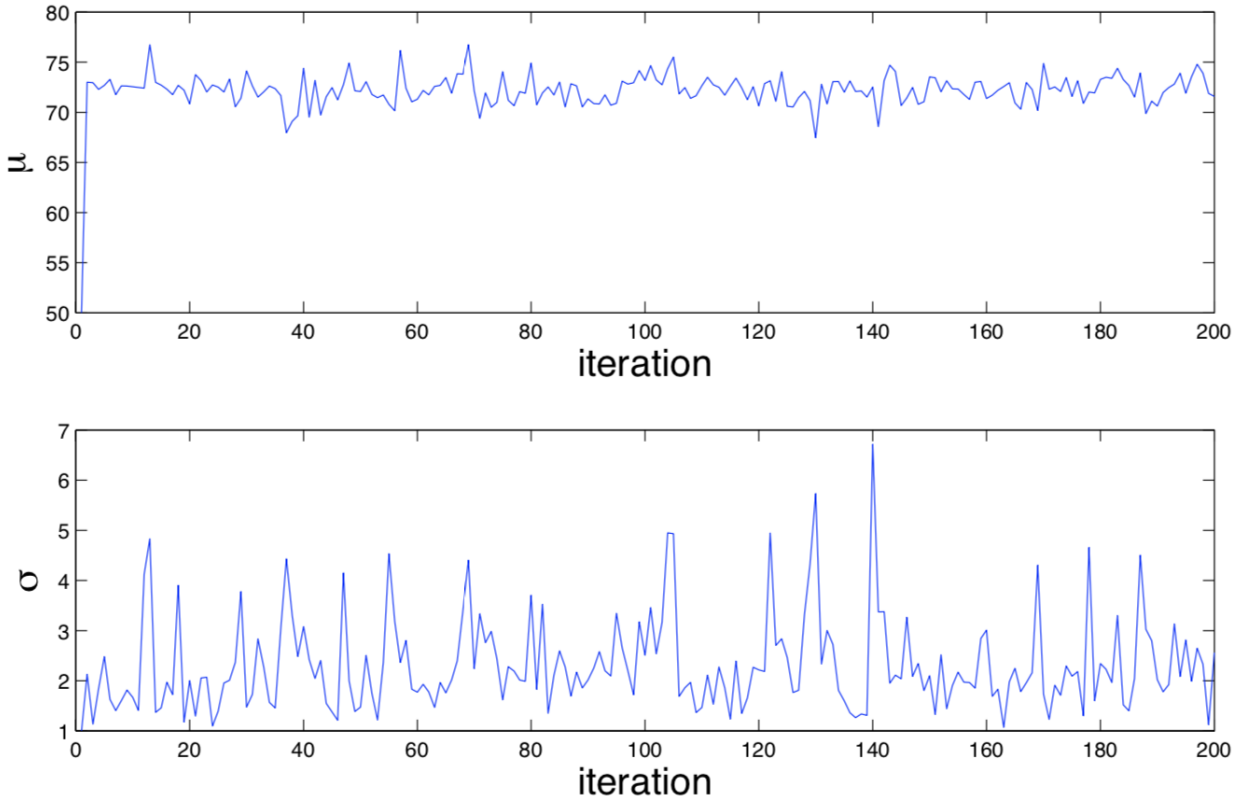
- Given $(\sigma^{(i)})^2$ at the i^{th} iteration, we sample $\mu^{(i+1)}$ from

$$\mu^{(i+1)} \sim \mathcal{N}\left(\frac{\frac{\mu_0}{\tau_0^2} + \frac{n\bar{y}}{(\sigma^{(i)})^2}}{\frac{1}{\tau_0^2} + \frac{n}{(\sigma^{(i)})^2}}, \frac{1}{\frac{1}{\tau_0^2} + \frac{n}{(\sigma^{(i)})^2}}\right)$$

- Given $\mu^{(i+1)}$, we sample a new σ^2 from

$$(\sigma^{(i+1)})^2 \sim \text{Inv-}\chi^2(\nu_0+n, \frac{\nu_0\sigma_0^2 + \nu n}{\nu_0 + n}), \quad \nu = \frac{1}{n}\sum_{j=1}^{n}(y_j - \mu^{(i+1)})^2$$

- The following graphs show the trace plots of the posterior samples (for both μ and σ)

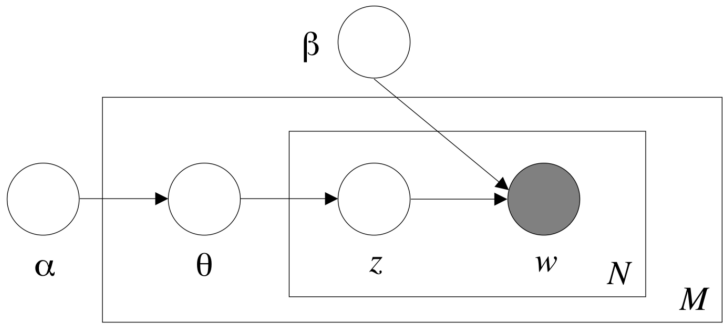


Gibbs sampling algorithms have been widely used in **probabilistic graphical models**

- Conditional distributions are fairly easy to derive for many graphical models (e.g., mixture models, Latent Dirichlet allocation)
- Have reasonable computation and memory requirements, only needs to sample one random variable at a time
- Can be Rao-Blackwellized (integrate out some random variable) to decrease the sampling variance. This is called *collapsed Gibbs sampling*

Example: Latent Dirichlet Allocation

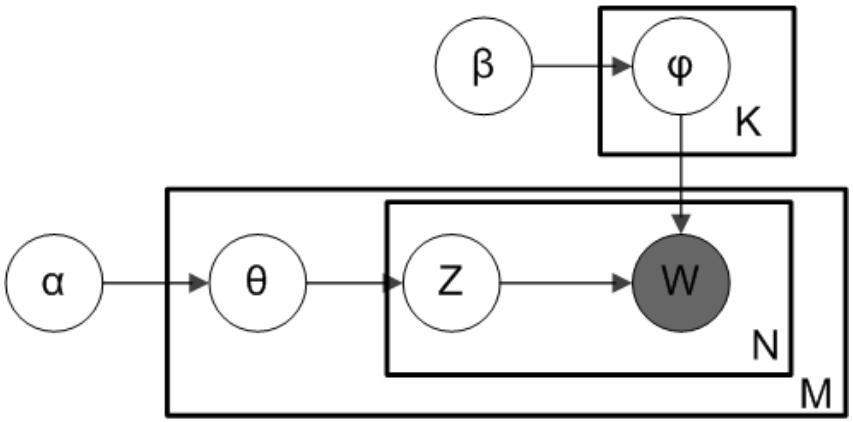
- Generative model of documents (Blei, Jordan and Ng, 2003). Also broadly applicable to collaborative filtering, image retrieval, bioinformatics, etc.



- choose a mixture of topics the document: $\theta \sim \text{Dir}(\alpha)$
- choose a topic for each of the document:

$$z_n \sim \text{Multinomial}(\theta)$$

- choose word given the topic: $w_n|z_n, \beta \sim p(w_n|z_n, \beta)$



- Use the probability model for LDA, with an additional Dirichlet prior on ϕ.
- The complete probability model

$$
\begin{aligned}
w_i|z_i, \phi^{(z_i)} &\sim \text{Discrete}(\phi^{(z_i)}) \\
\phi &\sim \text{Dirichlet}(\beta) \\
z_i|\theta^{(d_i)} &\sim \text{Discrete}(\theta^{(d_i)}) \\
\theta &\sim \text{Dirichlet}(\alpha)
\end{aligned}
$$

- The joint probability is

$$p(w, z, \phi, \theta|\alpha, \beta) = \prod_i p(w_i|z_i, \phi^{(z_i)})p(\phi|\beta) \cdot \prod_i p(z_i|\theta^{(d_i)})p(\theta|\alpha)$$

- Due to conjugate priors, we can easily integrate out ϕ and θ (T. Griffiths & M. Steyvers, 2004)

$$p(w|z) = \left(\frac{\Gamma(V\beta)}{\Gamma(\beta)^V}\right)^K \prod_{j=1}^K \frac{\prod_w \Gamma(n_j^{(w)} + \beta)}{\Gamma(n_j^{(\cdot)} + V\beta)}$$

$$p(z) = \left(\frac{\Gamma(K\alpha)}{\Gamma(\alpha)^K}\right)^M \prod_{d=1}^M \frac{\prod_j \Gamma(n_j^{(d)} + \alpha)}{\Gamma(n_\cdot^{(d)} + K\alpha)}$$

$n_j^{(w)} \leftarrow$ number of times word w assigned to topic j

$n_j^{(d)} \leftarrow$ number of times topic j used in document d

- Need full conditional distributions for variables
- We only sample z, whose conditional distributions is

$$p(z_i = j|z_{-i}, w) \propto \frac{n^{(w_i)}_{-i,j}+\beta}{n^{(\cdot)}_{-i,j}+V\beta} \frac{n^{(d_i)}_{-i,j}+\alpha}{n^{(d_i)}_{-i,\cdot}+K\alpha}$$

Gibbs Sampling

- Need full conditional distributions for variables
- We only sample z, whose conditional distributions is

$$p(z_i = j | z_{-i}, w) \propto \frac{n_{-i,j}^{(w_i)} + \beta}{n_{-i,j}^{(\cdot)} + V\beta} \frac{n_{-i,j}^{(d_i)} + \alpha}{n_{-i,\cdot}^{(d_i)} + K\alpha}$$

probability of w_i under topic j

Gibbs Sampling

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probability of w_i under topic j

probability of topic j in document d_i

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probability of w_i under topic j

probability of topic j in document d_i

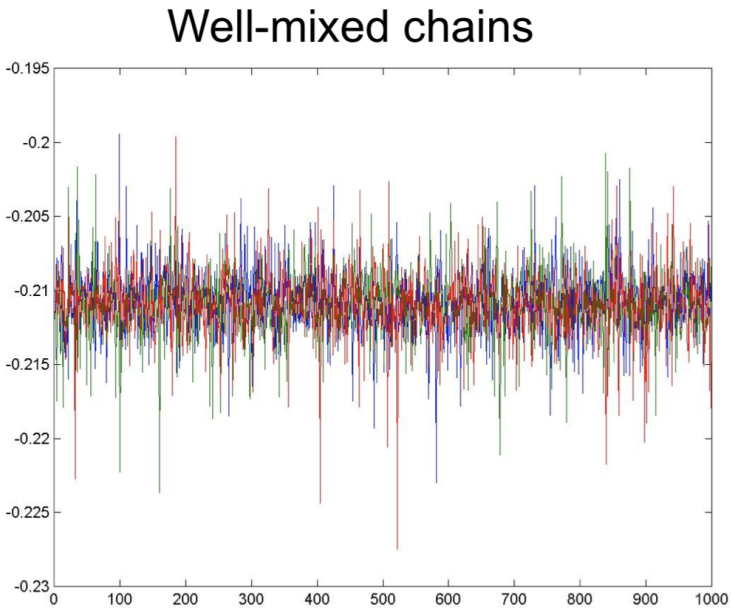
- This is nicer than your average Gibbs sampler:
  - memory: counts can be cashed in two sparse matrices
  - the distributions on ϕ and θ are analytic given z and w, and can later be found for each sample

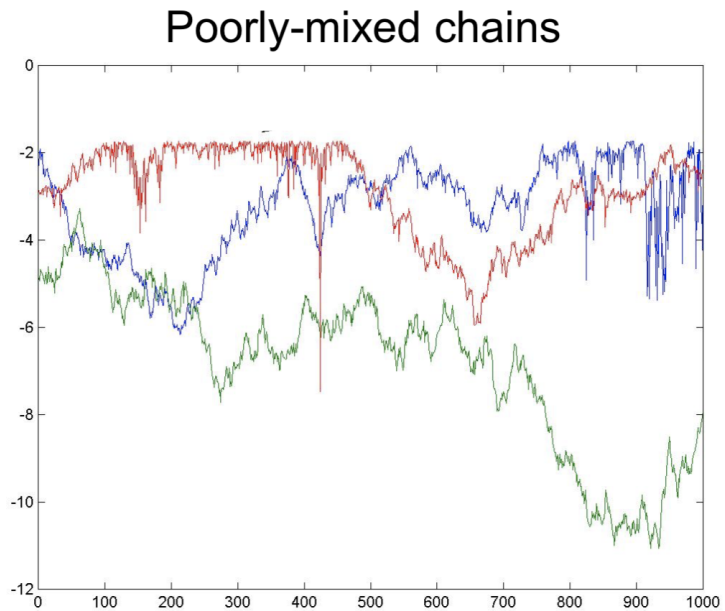
Combining Metropolis with Gibbs

- For more complex models, we might only have conditional conjugacy for one part of the parameters
- In such situations, we can combine the Gibbs sampler with the Metropolis method
- That is, we update the components with conditional conjugacy using Gibbs sampler and for the rest parameters, we use the Metropolis (or MH)

- MCMC would converge to the target distribution if run sufficiently long
- However, it is often non-trivial to determine whether the chain has converged or not in practice
- Also, how do we measure the efficiency of MCMC chains?
- In what follows, we will discuss some practical advice for coding MCMC algorithms

Graphical Diagnostics: Mixing Rate

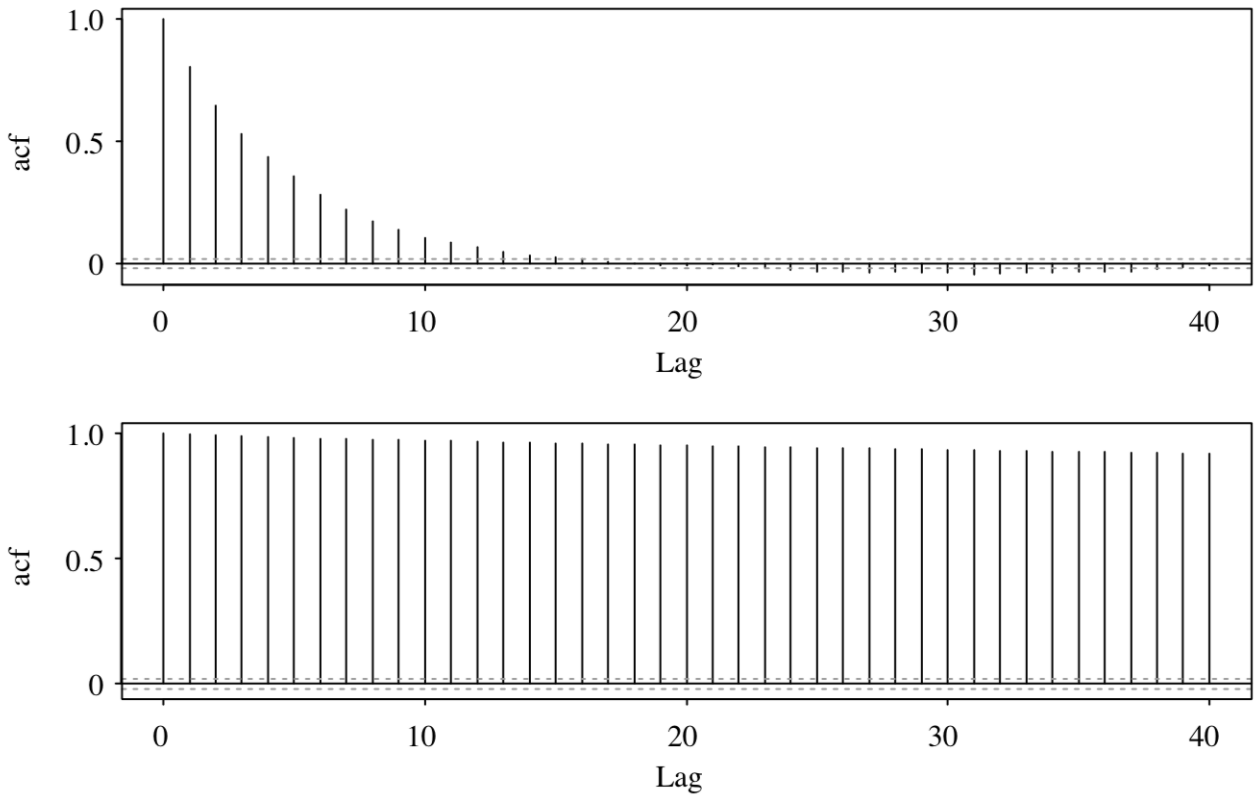




Monitor convergence by plotting samples from multiple MH runs (chains)

- If the chains are well-mixed (left), they are probably converged
- If the chains are poorly-mixed (right), we may need to continue burn-in

Graphical Diagnostics: Autocorrelation



- An autocorrelation plot summarizes the correlation in the sequence of a Markov chain at different iteration lags
- A chain that has poor mixing will exhibit slow decay of the autocorrelation as the lag increases

- Since MCMC samples are correlated, *effective sample size* are often used to measure the efficiency when MCMC samples are used for estimation instead of independent samples
- The effective sample size (ESS) is defined as

$$\text{ESS} = \frac{n}{1 + 2\sum_{k=1}^{\infty} \rho(k)}$$

  where $\rho(k)$ is the autocorrelation at lag k
- ESS are commonly used to compare the efficiency of competing MCMC samplers for a given problem. Larger ESS usually means faster convergence

Multiple Chains

- One of the hardest problem to diagnose is whether or not the chain has become stuck in one or more modes of the target distribution
- In this case, all convergence diagnostics may indicate that the chain has converged, though it does not
- A partial solution: run multiple chains and compare the within- and between-chain behavior

- Auxiliary variable strategies can be used to improving mixing of Markov chains
- When standard MCMC methods mix poorly, one potential remedy is to augment the state space of the variable of interest
- This approach can lead to chains that mix faster and require less tuning than the standard MCMC methods
- Main idea: construct a Markov chain over (X, U) (U is the auxiliary variable) with stationary distribution marginalizes to the target distribution of X
- As we will see later, this includes a large family of modern MCMC methods

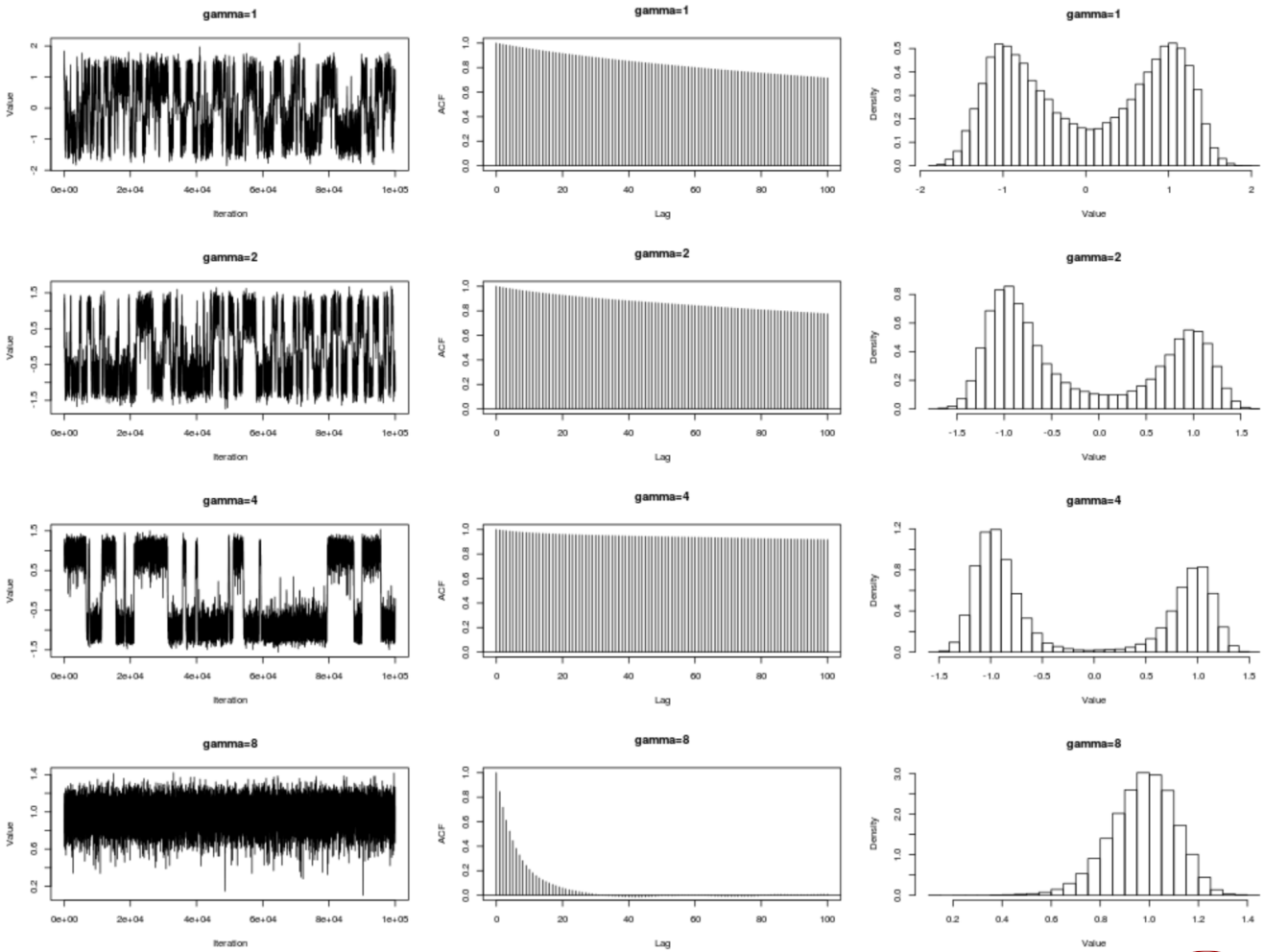
- Suppose that we have a challenging target distribution $f(x) \propto \exp(-U(x))$
- We can introduce temperatures to construct a sequence of distributions that are easier to sample from

$$f_k(x) \propto \exp\left(-U(x)/T_k\right), \quad k = 0, \ldots, K$$

  where $1 = T_0 < T_1 < \ldots < T_K$
- When simulating Markov chains with different temperature T, the chain with high temperature (hot chain) is likely to mix better than the chain with cold temperature (cold chain)
- Therefore, we can run parallel chains and swap states between the chains to improve mixing

Double-well Potential Distribution

$$f_T(x) \propto \exp(-(x^2-1)^2/T), \quad T = 1/\gamma$$



We run parallel Markov chains for distributions with different temperatures. In each iteration

- Follow regular Metropolis steps in each chain to get new states $x_0^{(t)}, \ldots, x_K^{(t)}$
- Select two temperatures, say $(i, j), i < j$, and swap the states

$$x_0^{(t)}, \ldots, x_i^{(t)}, \ldots, x_j^{(t)}, \ldots x_K^{(t)} \to x_0^{(t)}, \ldots, x_j^{(t)}, \ldots, x_i^{(t)}, \ldots x_K^{(t)}$$

- Accept the swapped new states with the following probability

$$\min\left(1, f_i(x_j^{(t)}) f_j(x_i^{(t)}) / f_i(x_i^{(t)}) f_j(x_j^{(t)})\right)$$

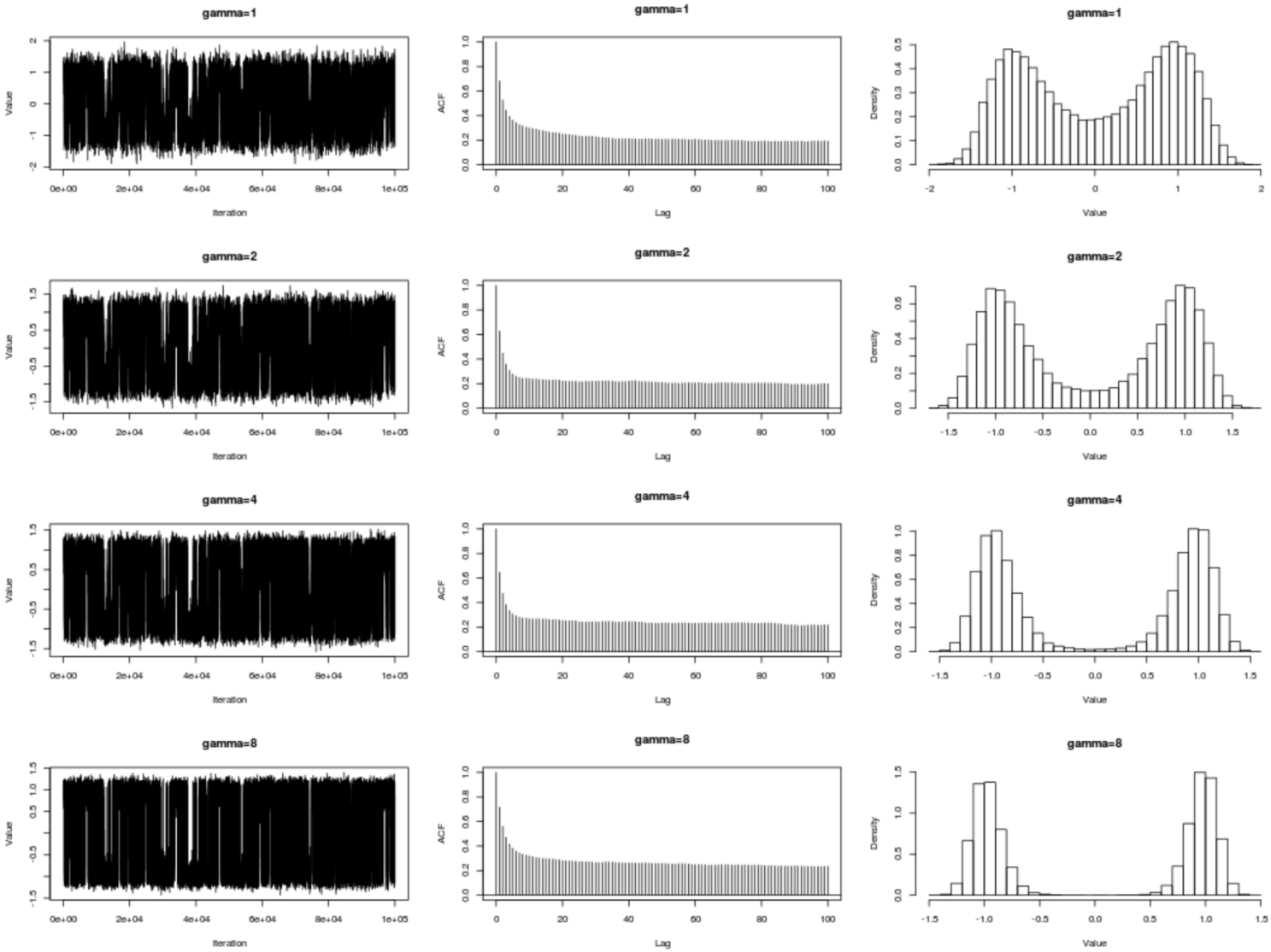
Parallel Tempering

- Both the within-chain Metropolis updates and the between-chain swap preserves

$$p(x_0, \ldots, x_K) \propto f_0(x_0) f_1(x_1) \ldots f_K(x_K)$$

- Therefore, the joint distribution of $(x_0^{(t)}, \ldots, x_K^{(t)})$ will converge to $p(x)$, and the marginal distribution of x_0 (cold chain) is the target distribution
- There are many ways to swap chains. For example, we can pick a pair of temperatures uniformly at random or only swap chains with successive temperatures
- The design of temperature levels could be crucial for the performance

Example: Double-well Potential Distribution



- Slice sampling was introduced by Neal (2003) to accelerate mixing of Metropolis (or MH)
- It is essentially a Gibbs sampler in the augmented space (X, U) with density

$$f(x, u) = f(x)f(u|x)$$

where U is the auxiliary variable and $f(u|x)$ is designed to be a uniform distribution $\mathcal{U}(0, f(x))$

- For this purpose, slice sampling alternates between two steps:
  - Given the current state of the Markov chain, x, we uniformly sample a new point u from the interval $(0, f(x))$

$$U|x \sim \mathcal{U}(0, f(x))$$

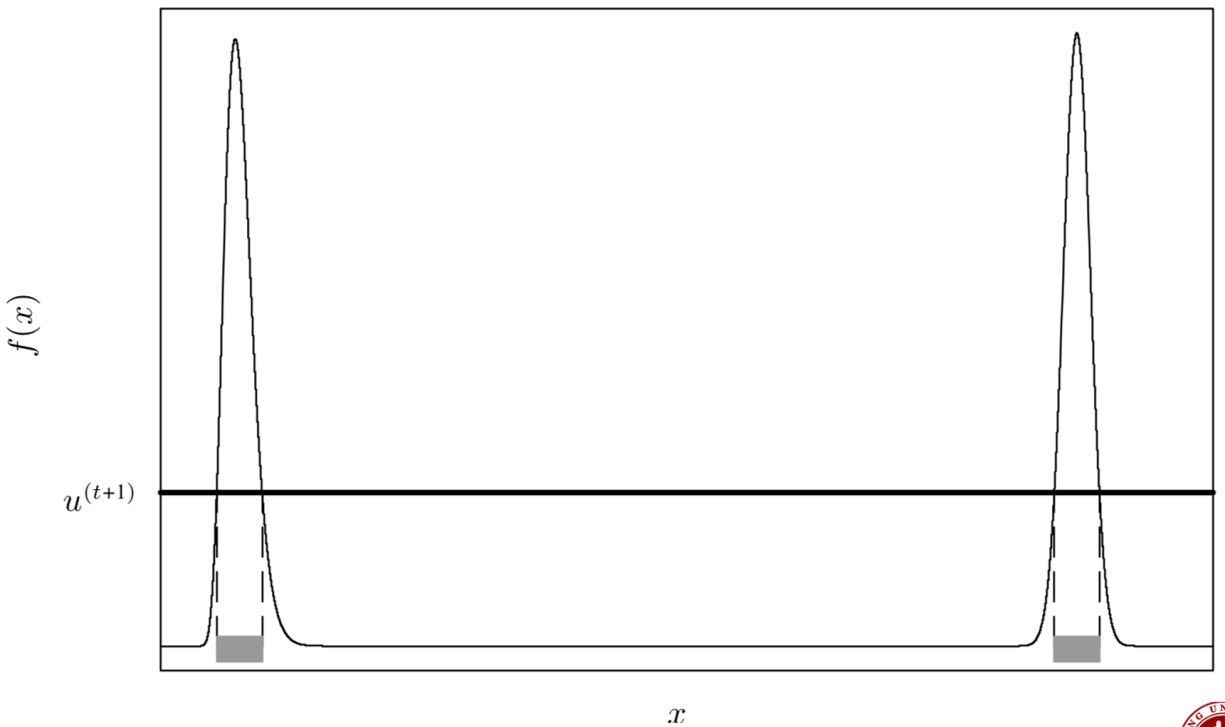
  - Given the current value of u, we uniformly sample from the region $S = \{x : f(x) > u\}$, which is referred to as the *slice* defined by u

$$X|u \sim \mathcal{U}(S)$$

- As mentioned by Neal (2003), in practice it is safer to compute $g(x) = \log(f(x))$, and use the auxiliary variable $z = \log(u) = g(x) - e$, where e has exponential distribution with mean one, and define the slice as $S = \{x : z < g(x)\}$

Move Between Modes with Slice Sampler

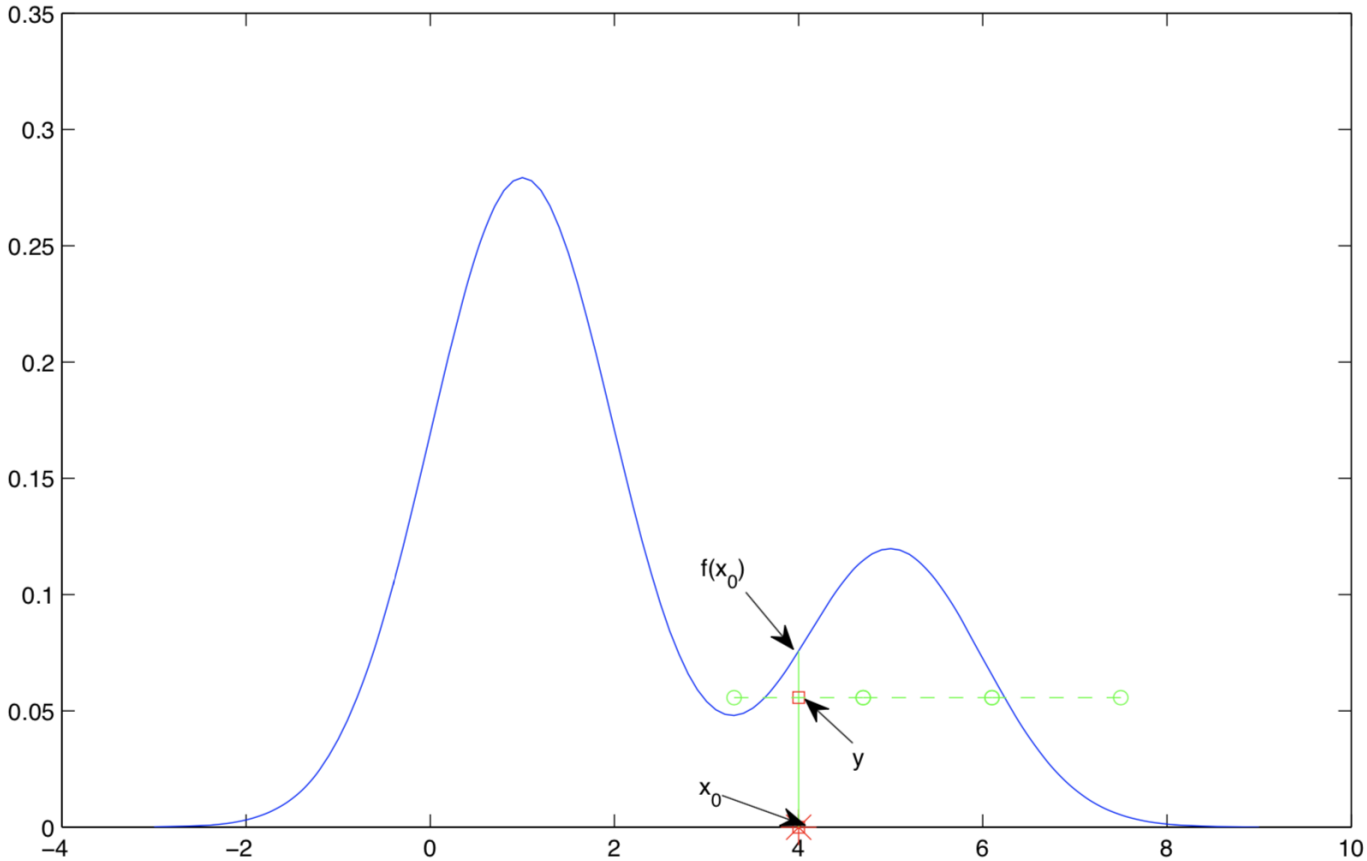
- One advantage of slice sampling is for sampling from multimodal distributions
- Unlike standard Metropolis (or MH) that struggles between distant modes, sampling from the slice allows us to easily jump between different modes



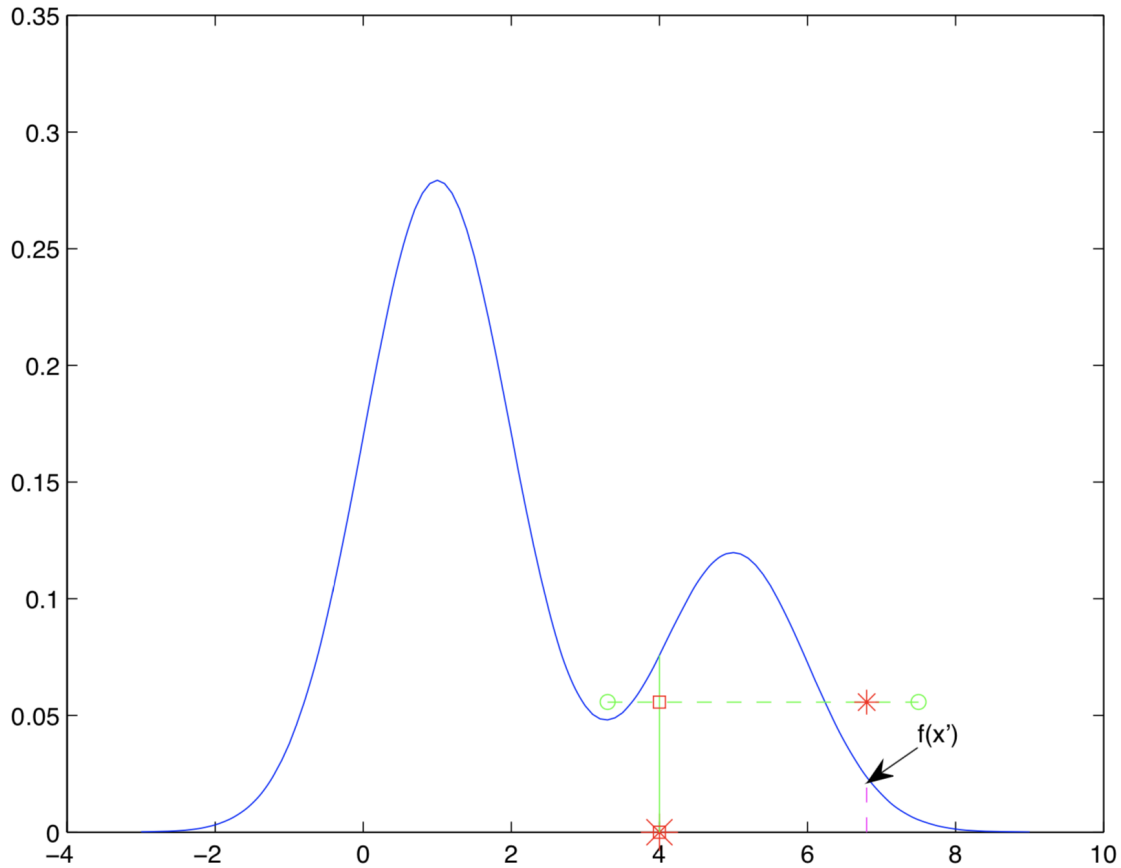
- Sampling an independent point uniformly from S might be difficult. In practice, we can substitute this step by any update that leaves the uniform distribution over S invariant
- There are several methods to perform this task
- Here, we introduce a simple but effective procedure that consists of two phases:
  - *Stepping-out*. A procedure for finding an interval around the current point
  - *Shrinkage*. A procedure for sampling form the interval obtained
- For a detail description of these methods, see Neal (2003)

Slice Sampling- Illustration

- Sampling $u \sim \mathcal{U}(0, f(x_0))$ and stepping out (of size w) until we reach points outside the slice

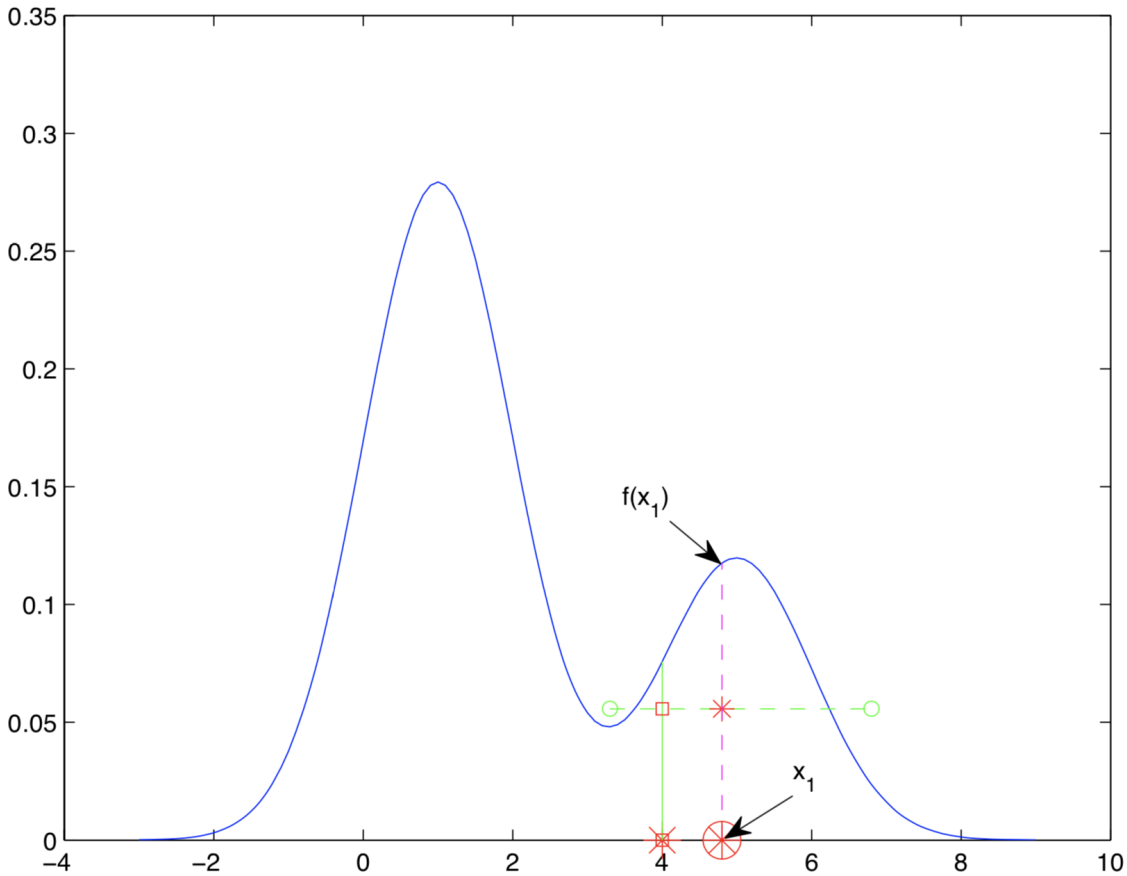


- Shrinkage of interval to a point, x', which is sampled (uniformly) from the interval but it has $f(x') < y$



Slice Sampling- Illustration

- Continue shrinkage until we reach a point x_1 such that $y < f(x_1)$. We accept x_1 as our new sample



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