

Bayesian Theory and Computation

Lecture 4: Markov Chain Monte Carlo I



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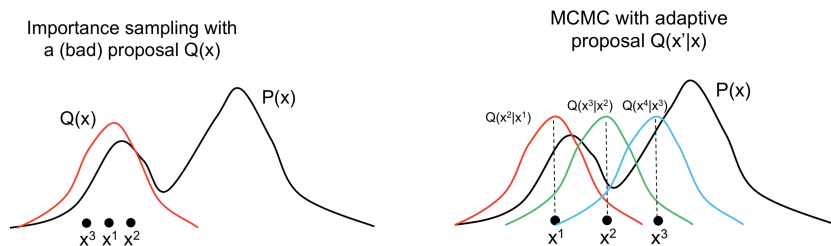
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- ▶ Now suppose we are interested in sampling from a distribution π (e.g., the unnormalized posterior)
- ▶ Markov chain Monte Carlo (MCMC) is a method that samples from a Markov chain whose stationary distribution is the target distribution π . It 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

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

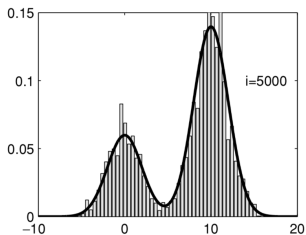
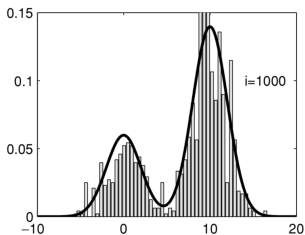
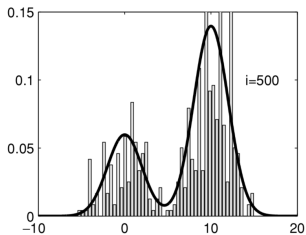
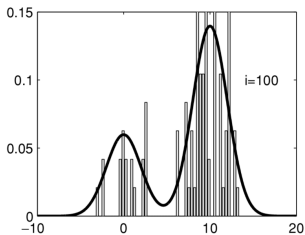
In each iteration we do the following

- ▶ 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 $\pi(x)$



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

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



- ▶ 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

- ▶ 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

- ▶ Recall the univariate Gaussian model with known variance

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

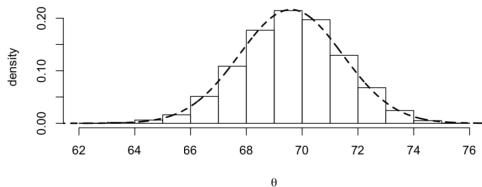
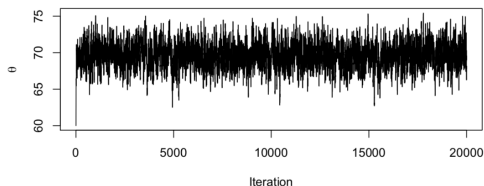
- ▶ Note that there is a conjugate $\mathcal{N}(\mu_0, \tau_0^2)$ prior for θ , and the posterior has a close form normal distribution
- ▶ Now let's pretend that we don't know this exact posterior distribution and use a Markov chain to sample from it.

- ▶ 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

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



- ▶ Recall the binomial model:

$$p(y|n, \theta) = \binom{n}{y} \theta^y (1 - \theta)^{n-y}$$

- ▶ Assuming the conjugate prior $\text{Beta}(\alpha, \beta)$ for θ , we saw that the posterior is $\text{Beta}(\alpha + y, \beta + n - y)$.
- ▶ For the election example, we mentioned that out of 100 people surveyed, 39 said they are going to vote for A . We used a conjugate $\text{Beta}(1, 1)$ prior and obtained $\text{Beta}(40, 62)$ as the posterior distribution for θ .
- ▶ Now let's not use the closed form of the posterior distribution and use the Metropolis algorithm instead.

- ▶ We first need to find the posterior distribution (up to a constant).
- ▶ The prior distribution is of course uniform: $p(\theta) = 1$.
- ▶ The likelihood is (ignore the irrelevant constant)

$$p(y|\theta) \propto \theta^y(1 - \theta)^{n-y}$$

where $n = 100$ and $y = 39$.

- ▶ Therefore, using the Bayes' theorem, the posterior is

$$p(\theta|y) \propto p(\theta)p(y|\theta) \propto \theta^{39}(1 - \theta)^{61} = P(\theta)$$

- ▶ Next, we need to choose a transition (i.e., proposal) distribution.
- ▶ Let's use $\text{Uniform}(0, 1)$. This is of course symmetric.
- ▶ Now we start from $x_0 = 0.5$ and repeat the following steps
 - ▶ sample θ' from $\text{Uniform}(0, 1)$
 - ▶ calculate the acceptance probability

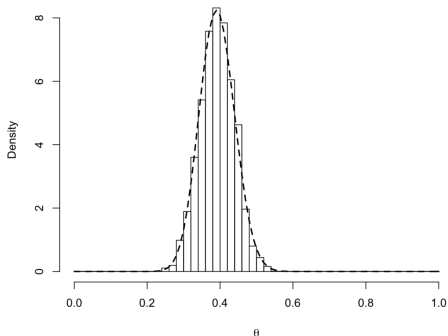
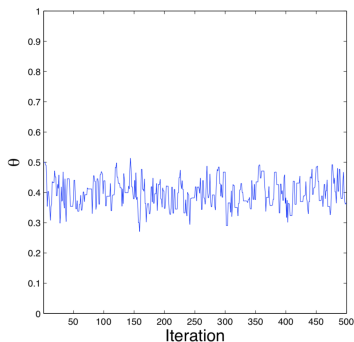
$$a(\theta'|\theta^{(i)}) = \min\left(1, \frac{(\theta')^{39}(1-\theta')^{61}}{(\theta^{(i)})^{39}(1-\theta^{(i)})^{61}}\right)$$

- ▶ Accept the proposed value with probability $a(\theta'|\theta)$. For this, we can sample $u \sim \text{Uniform}(0, 1)$ and set

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



Trace plot and posterior estimation



- ▶ Recall the Beckham's example. We modeled the number of goals y_i he scores in a game using a Poisson model

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

- ▶ He scored 0 and 1 goals in the first two games respectively
- ▶ We used $\text{Gamma}(1.4, 10)$ 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

- ▶ 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

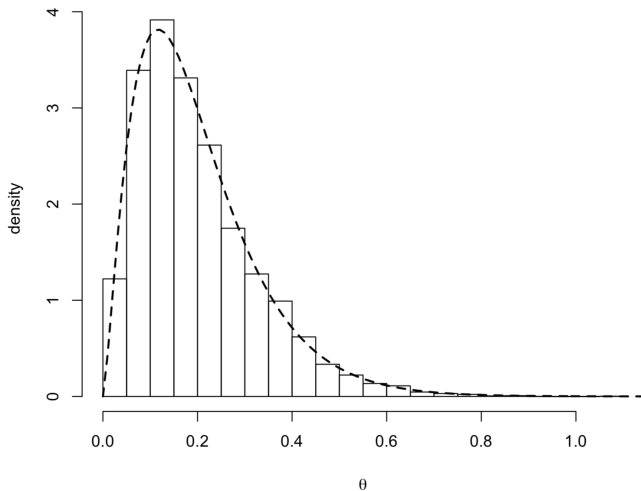
- ▶ Sample θ' from $\mathcal{U}(0, \theta^{(i)} + 1)$
- ▶ Calculate the acceptance probability

$$a(\theta'|\theta^{(i)}) = \min \left(1, \frac{P(\theta')\text{Uniform}(\theta^{(i)}|0, \theta' + 1)}{P(\theta^{(i)})\text{Uniform}(\theta'|0, \theta^{(i)} + 1)} \right)$$

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

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





- ▶ What if the distribution is multidimensional, *i.e.*,
 $x = (x_1, x_2, \dots, x_d)$
- ▶ We can still use the Metropolis algorithm (or MH), with a multivariate proposal distribution, *i.e.*, we now propose
 $x' = (x'_1, x'_2, \dots, x'_d)$
- ▶ 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

- ▶ 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

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

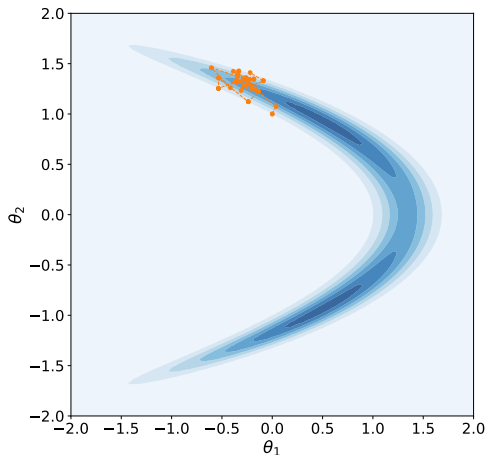
- ▶ The posterior is

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

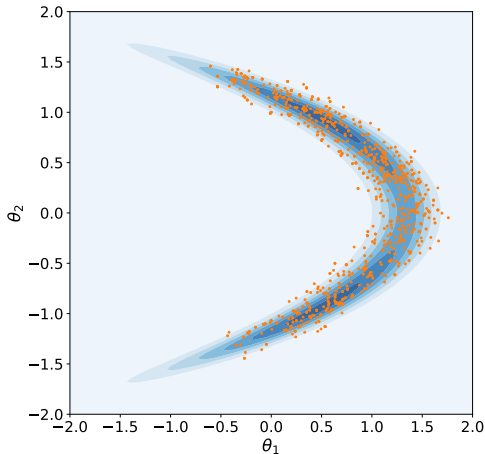
- ▶ We use the Metropolis algorithm to sample from posterior, with a bivariate normal proposal distribution such as $\mathcal{N}(\theta^{(i)}, (0.15)^2 I)$



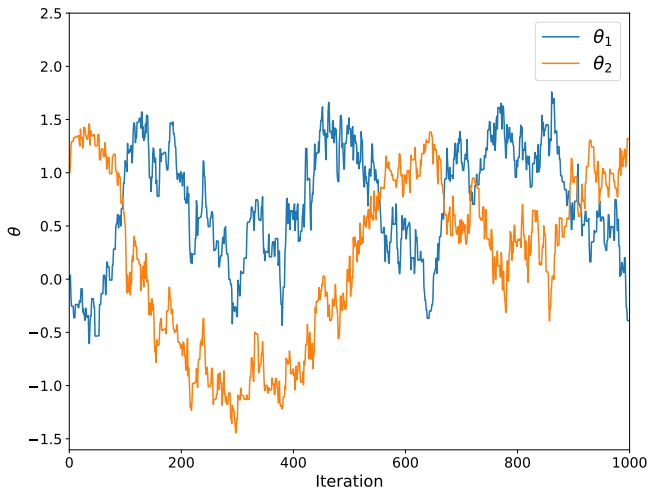
The first few samples from the posterior distribution of $\theta = (\theta_1, \theta_2)$, using a bivariate normal proposal



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



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



- ▶ 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 $(x_1^{(i)}, \dots, x_d^{(i)})$, we do the following for all components $k = 1, 2, \dots, d$
 - ▶ Sample x'_k from the univariate proposal distribution $Q(x'_k | \dots, x_{k-1}^{(i+1)}, x_k^{(i)}, \dots)$
 - ▶ Accept this new value and set $x_k^{(i+1)} = x'_k$ with probability

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

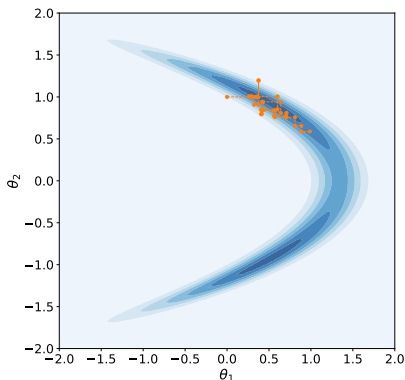
or reject it and set $x_k^{(i+1)} = x_k^{(i)}$



- ▶ 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



- ▶ 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 works as follows
- ▶ Initialize starting value for x_1, x_2, \dots, x_d
- ▶ At each iteration, pick an ordering of the d variables (can be sequential or random)
 1. Sample $x \sim P(x_i | x_1, \dots, x_{i-1}, x_{i+1}, \dots, x_d)$, *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 its new value for sampling other variables x_j

- ▶ 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

$$\begin{aligned} a(x'_i, x_{-i} | x_i, x_{-i}) &= \min \left(1, \frac{P(x'_i, x_{-i})Q(x_i, x_{-i} | x'_i, x_{-i})}{P(x_i, x_{-i})Q(x'_i, x_{-i} | x_i, x_{-i})} \right) \\ &= \min \left(1, \frac{P(x'_i, x_{-i})P(x_i | x_{-i})}{P(x_i, x_{-i})P(x'_i | x_{-i})} \right) = \min \left(1, \frac{P(x'_i, x_{-i})P(x_i, x_{-i})}{P(x_i, x_{-i})P(x'_i, x_{-i})} \right) \\ &= 1 \end{aligned}$$



- ▶ 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

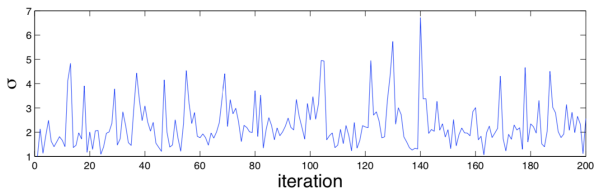
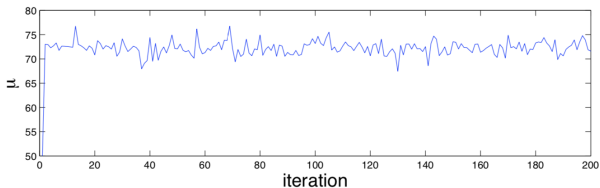
$$\mu^{(i+1)} \sim \mathcal{N}\left(\frac{\frac{\mu_0}{\tau_0^2} + \frac{n\bar{y}}{(\sigma^{(i)})^2}}{\frac{1}{\tau_0^2} + \frac{n}{(\sigma^{(i)})^2}}, \frac{1}{\frac{1}{\tau_0^2} + \frac{n}{(\sigma^{(i)})^2}}\right)$$

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

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



- ▶ 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*
- ▶ We will see examples later.

- ▶ 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)

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- ▶ Hastings, W.K. (1970). Monte Carlo sampling methods using Markov chains and their applications. *Biometrika* 57, 97–109.
- ▶ Geman, S. and Geman, D. (1984). Stochastic relaxation, Gibbs distributions, and the Bayesian restoration of images. *IEEE Transactions on Pattern Analysis and Machine Intelligence* 6, 721–741.
- ▶ Andrieu, C., De Freitas, N., Doucet, A. and Jordan, M. I. (2003). An introduction to MCMC for machine learning. *Machine learning* 50, 5–43.