Statistical Models & Computing Methods

Lecture 4: Markov Chain Monte Carlo

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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**.

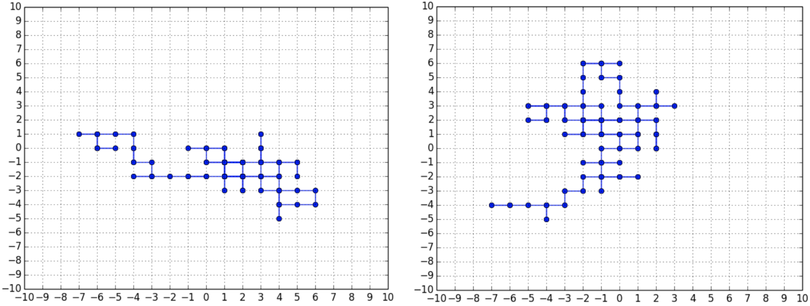
- Stochastic processes is a family of random variables, usually indexed by a set of numbers (time). A discrete time stochastic process is simply a sequence of random variables, $X_0, X_1, \ldots, X_n$ defined on the same probability space
- One of the simplest stochastic processes (and one of the most 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

Markov Property

- 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

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

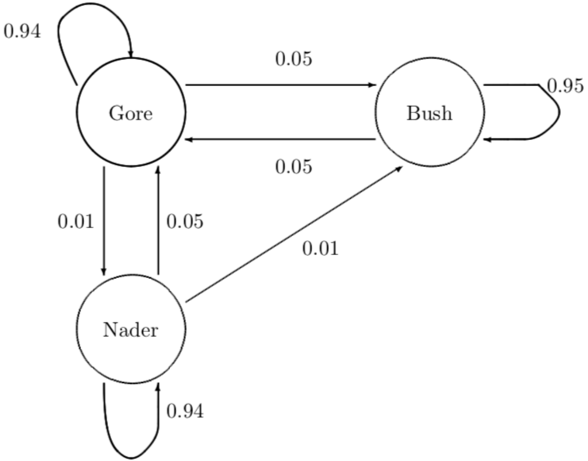
fully determined by the transition probabilities

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

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 vs. Transient

- **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 $\sum_i p_{ji} = 1$ 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

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

- 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. $x \in \mathcal{X}$,

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

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

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

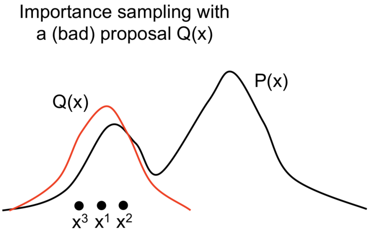
In particular, π is the unique stationary probability density function for the chain

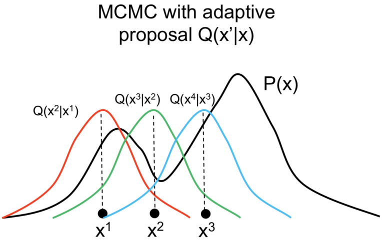
Markov chain Monte Carlo

- 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

Markov chain Monte Carlo

- 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

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

The Metropolis Algorithm

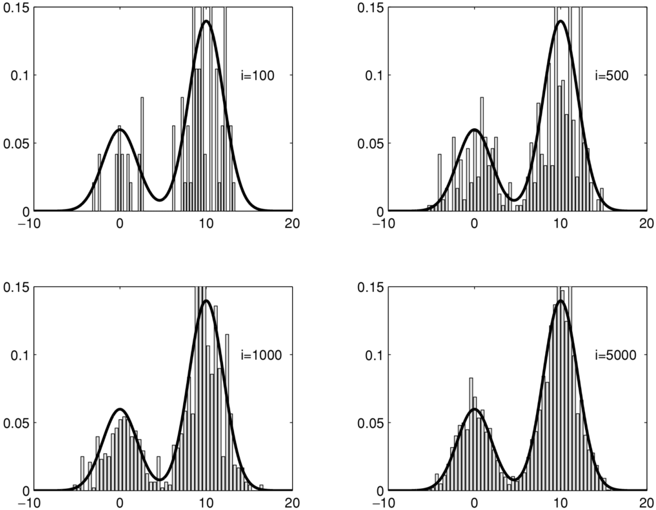
In each iteration we do the following

- 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

- Recall the univariate Gaussian model with known variance

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

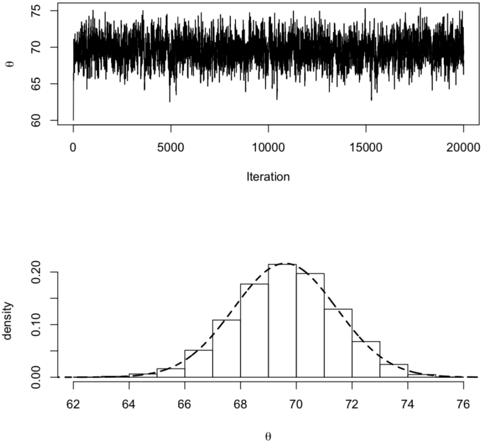
- Note that there is a conjugate $\mathcal{N}(\mu_0, \tau_0^2)$ prior for θ, and the posterior has a close form normal distribution
- Now let's pretend that we don't know this exact posterior distribution and use a Markov chain to sample from it.

- 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



- 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 $\text{Gamma}(1.4, 10)$ 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

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

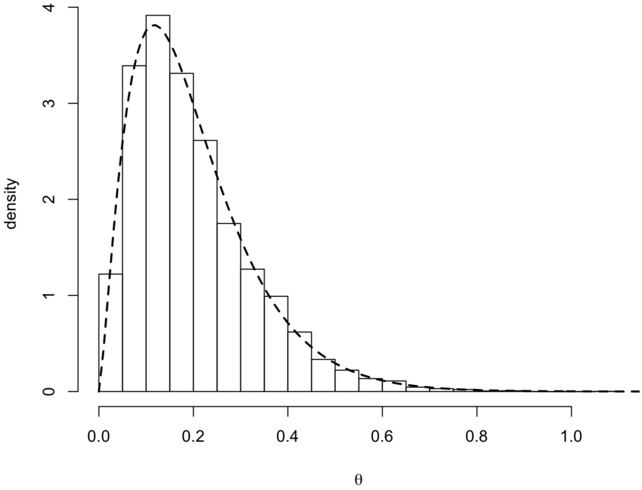
- Sample θ' from $\mathcal{U}(0, \theta^{(i)} + 1)$
- Calculate the acceptance probability

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

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

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

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

- 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

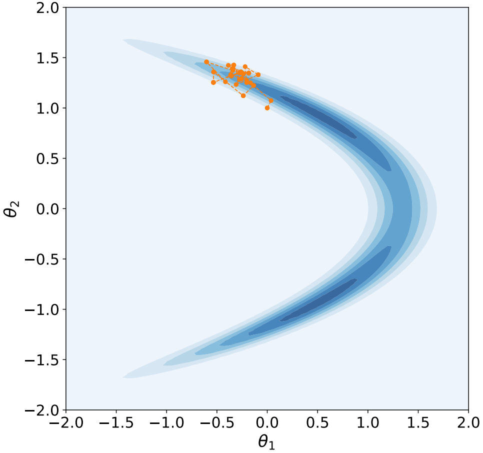
$$\theta = (\theta_1, \theta_2) \sim \mathcal{N}(0, I)$$

- The posterior is

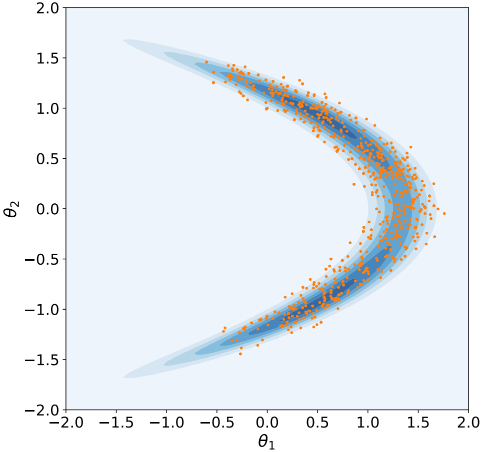
$$p(\theta|y) \propto \exp\left(-\frac{\theta_1^2 + \theta_2^2}{2}\right) \cdot \exp\left(-\frac{\sum_i (y_i - \theta_1 - \theta_2^2)^2}{2\sigma_y^2}\right)$$

- 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

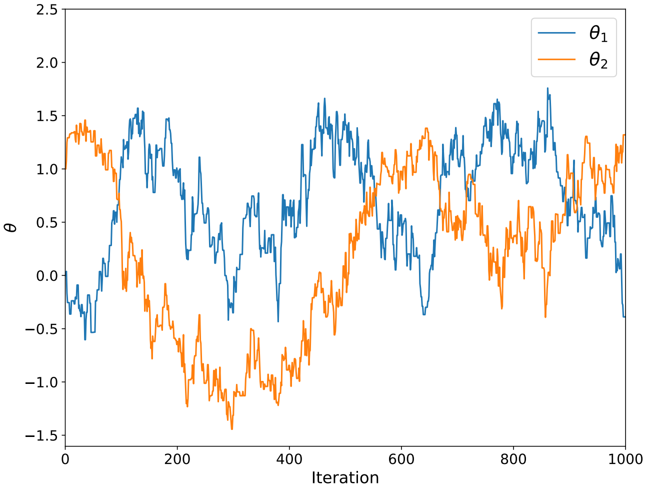


Posterior samples for $\theta = (\theta_1, \theta_2)$



Examples: Banana Shape Distribution

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 $(x_1^{(i)}, \ldots, x_d^{(i)})$, 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

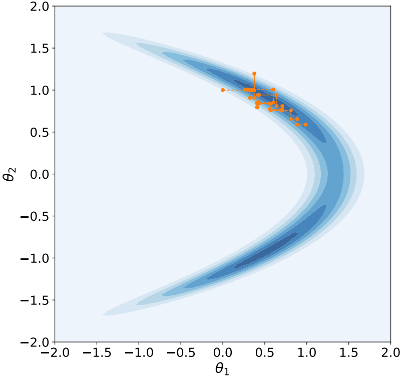
$$a(x'_k | \ldots, x_{k-1}^{(i+1)}, x_k^{(i)}, \ldots)) = \min\left(1, \frac{P(\ldots, x_{k-1}^{(i+1)}, x'_k, \ldots)}{P(\ldots, x_{k-1}^{(i+1)}, x_k^{(i)}, \ldots)}\right)$$

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

- 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

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

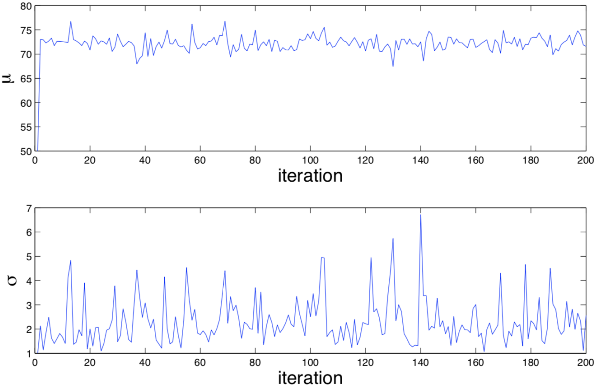
- Given $(\sigma^{(i)})^2$ at the i^{th} iteration, we sample $\mu^{(i+1)}$ from

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

- 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 known as *collapsed Gibbs sampling*.

- Energy-based models (EBMs) associate a scalar energy to each configuration of the variables of interest
- We can modify the energy function so that its shape has desirable properties, e.g., plausible configurations would have lower energy
- Energy-based probabilistic models define a probability distribution through an energy function as follows

$$p(x) = \frac{1}{Z}\exp(-E(x)), \quad Z = \sum_x \exp(-E(x))$$

- EBMs can be learnt by maximizing the log-likelihood using stochastic gradient

$$-\frac{\partial \log p_\theta(x)}{\partial \theta} = \frac{\partial E_\theta(x)}{\partial \theta} - \mathbb{E}_{x\sim p_\theta(x)}\frac{\partial E_\theta(x)}{\partial \theta}$$

- In many cases, we do not have full observation, or we want to introduce latent variables to increase model capacity

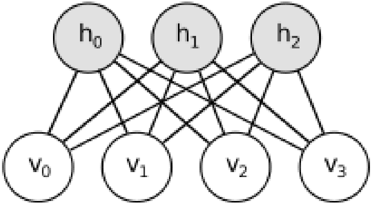
$$p(x) = \sum_h p(x,h) = \frac{1}{Z}\sum_h \exp(-E(x,h)) \tag{1}$$

- We can define free energy to turn (1) into a *regular* EBM

$$p(x) = \frac{1}{Z}\exp(-\mathcal{F}(x)), \quad \mathcal{F}(x) = -\log\sum_h \exp(-E(x,h))$$

- An interesting form for the gradient

$$\begin{aligned}-\frac{\partial \log p_\theta(x)}{\partial\theta} &= \frac{\partial \mathcal{F}_\theta(x)}{\partial\theta} - \mathbb{E}_{x\sim p_\theta(x)}\frac{\partial \mathcal{F}_\theta(x)}{\partial\theta}\\ &= \mathbb{E}_{h\sim p_\theta(h|x)}\frac{\partial E_\theta(x,h)}{\partial\theta} - \mathbb{E}_{x,h\sim p_\theta(x,h)}\frac{\partial E_\theta(x,h)}{\partial\theta}\end{aligned}$$



- Restricted Boltzmann Machines (RBMs) are a particular form of EBMs where the energy function is a bilinear function of the visible and hidden variables

$$E(v, h) = -b^T v - c^T h - h^T W v$$

- The visible and hidden units are conditionally independent

$$p(h|v) = \prod_i p(h_i|v), \quad p(v|h) = \prod_j p(v_j|h)$$

- When v and h are binary variables, we have

$$p(h_i = 1|v) = \text{sigmoid}(c_i + W_i v), \; p(v_j = 1|h) = \text{sigmoid}(b_j + W_j^T h)$$

- Use Gibbs sampling for training and sampling

$$h^{(n+1)} \sim \text{Bernoulli}\left(\text{sigmoid}(c + Wv^{(n)})\right)$$
$$v^{(n+1)} \sim \text{Bernoulli}\left(\text{sigmoid}(b + W^T h^{(n+1)})\right)$$

- Contrastive Divergence:

$$-\frac{\partial \log p_\theta(v)}{\partial \theta} \approx \frac{\partial \mathcal{F}_\theta(v)}{\partial \theta} - \frac{\partial \mathcal{F}_\theta(\tilde{v})}{\partial \theta}$$

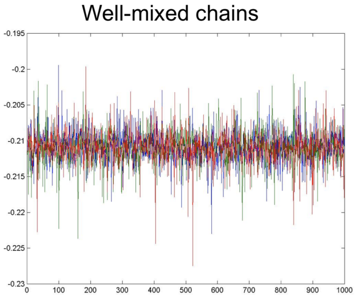
where $\tilde{v}$ is a sample from the MCMC chain after k steps *starting from the observed sample* v.

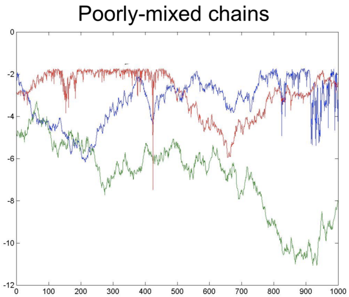
Combining Metropolis with Gibbs

- 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

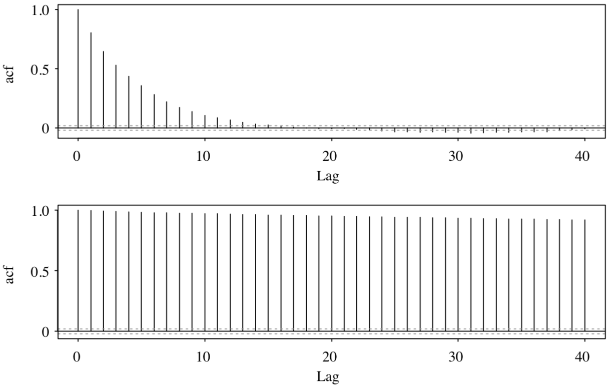




Monitor convergence by plotting samples from multiple MH runs (chains)

- 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

Effective Sample Size

- 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

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

  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

- Metropolis, N. (1953). Equation of state calculations by fast computing machines. The Journal of Chemical Physics 21, 1087–1092.
- 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.

References

- Yoshua Bengio. 2009. Learning deep architectures for AI. Foundations and Trends in Machine Learning.