Markov chain Monte Carlo



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Today we are going to learn...

Markov Chains

- 2 Metropolis Algorithm
- Metropolis-Hastings
- Multiple variables

Markov Chains

- The goal of today's lecture is to learn about the Metropolis Hastings algorithm
- The Metropolis Hastings algorithm allows us to simulate from any distribution as long as we have the kernel of the density of the distribution.
- To understand the Metropolis Hastings algorithm, we must learn a little bit about Markov chains

Basic Probability Rules

Law of conditional probability

$$Pr(A = a, B = b) = Pr(A = a|B = b)Pr(B = b)$$
(1)

More general conditional probability

$$Pr(A = a, B = b|C = c) = Pr(A = a|B = b, C = c) \times$$

$$Pr(B = b|C = c)$$
(2)

Basic Probability Rules

• Marginalizing (for a discrete variable)

$$Pr(A = a) = \sum_{b} Pr(A = a, B = b)$$
 (3)

More general

$$Pr(A = \alpha | C = c) = \sum_{b} Pr(A = \alpha, B = b | C = c)$$
 (4)

Independence

• Two variables are independent if

$$Pr(A = a, B = b) = Pr(A = a)Pr(B = b) \quad \forall a, b$$
 (5)

• Dividing both sides by Pr(B=b) gives

$$Pr(A = a|B = b) = Pr(A = a) \quad \forall a, b$$
 (6)

Conditional Independence

Two variables A and B are Conditionally Independent if

$$Pr(A = a, B = b | C = c) = Pr(A = a | C = c) \times$$

$$Pr(B = b | C = c) \quad \forall a, b, c$$
(7)

• Dividing both sides by Pr(B = b | C = c) gives

$$Pr(A = a|B = b, C = c) = Pr(A = a|C = c) \quad \forall a, b, c \tag{8}$$

A simple game

- Player A and Player B play a game. The probability that Player A wins each game is 0.6 and the probability that Player B wins each game is 0.4.
- They play the game N times.
- Each game is independent.
- Let
 - $X_i = 0$ if Player A wins game i
 - $X_i = 1$ if Player B wins game i
- Also assume there is an initial Game called Game 0 (X_0)

Some simple questions

- What is the probability that Player A wins Game 1 $((X_1 = 0))$ if
 - If $X_0 = 0$ (Player A wins Game 0)
 - If $X_0 = 1$ (Player B wins Game 0)
- What is the probability that Player A wins Game 2 $((X_2 = 0))$ if
 - If $X_0 = 0$ (Player A wins Game 0)
 - If $X_0 = 1$ (Player B wins Game 0)
- Since each game is independent all answers are 0.6.

A different game: A Markov chain

ullet Now assume that both players have a better chance of winning Game i+1 if they already won Game i.

$$Pr(X_{i+1} = 0 | X_i = 0) = 0.8$$
(9)

$$Pr(X_{i+1} = 1 | X_i = 1) = 0.7 \tag{10}$$

- Assume nothing other than game i has a direct effect on Game i+1.
- This is called the Markov Property. Mathematically

$$Pr(X_{i+1}|X_i, X_{i-1}, \dots, X_1, X_0) = Pr(X_{i+1}|X_i)$$
 (11)

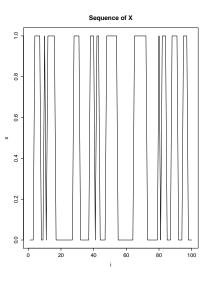
Markov Property

- Another way to define the Markov property is to notice that X_{i+1} and X_{i-1},\ldots,X_0 are **independent** conditional on X_i
- This may be a model for the stock market, all the valuable information about tomorrow's stock price is contained in today's price.
- This is related to the Efficient Market Hypothesis, a popular theory in finance
- Now back to the simple game.

Simulating from a Markov chain

- Now let's simulate a sequence $X_1, X_2, \ldots, X_{100}$ from the Markov chain.
- Initialize at $x_0 = 0$. Then inside a loop
- Code the following using *if*.
- Try it

Markov chain



Simple questions again

- What is the probability that Player A wins the first game (i.e $(X_1 = 0)$) if
 - If $X_0 = 0$ (Player A wins initial game)
 - If $X_0 = 1$ (Player B wins initial game)
- The answers are 0.8 and 0.3.
- What is the probability that Player A wins the second game $(X_2 = 0)$ if
 - If $X_0 = 0$ (Player A wins initial game)
 - If $X_0 = 1$ (Player B wins initial game)

Solution

• Let $X_0 = 0$. Then $Pr(X_2 = 0|X_0 = 0)$

$$\begin{split} &= \sum_{x_1=0,1} \mathsf{Pr}(X_2=0, X_1=x_1|X_0=0) \\ &= \sum_{x_1=0,1} \mathsf{Pr}(X_2=0|X_1=x_1, X_0=0) \mathsf{Pr}(X_1=x_1|X_0=0) \\ &= \sum_{x_1=0,1} \mathsf{Pr}(X_2=0|X_1=x_1) \mathsf{Pr}(X_1=x_1|X_0=0) \\ &= 0.8 \times 0.8 + 0.3 \times 0.2 \\ &= 0.7 \end{split}$$

• What if $X_0 = 1$?

Recursion

- Notice that the distribution of X_i depends on X₀
- The sequence is no longer independent.
- How could you compute $\text{Pr}(X_n=0|X_0=0)$ when n=3, when n=5, when n=100?
- This is hard, but the Markov Property does make things simpler
- We can use a recursion to compute the probability that Player A wins any game.

Recursion

Note that
$$Pr(X_i = 0|X_0 = 0)$$

$$\begin{split} &= \sum_{x_{i-1}} \Pr(X_i = 0, X_{i-1} = x_{i-1} | X_0 = 0) \\ &= \sum_{x_{i-1}} \Pr(X_i = 0 | X_{i-1} = x_{i-1}, X_0 = 0) \Pr(X_{i-1} = x_{i-1} | X_0 = 0) \\ &= \sum_{x_{i-1}} \Pr(X_i = 0 | X_{i-1} = x_{i-1}) \Pr(X_{i-1} = x_{i-1} | X_0 = 0) \end{split}$$

We already applied this formula when i=2. We can continue for $i=3,4,5,\ldots,n$

Recursion

$$\Pr(X_{\mathfrak{i}} = 0 | X_0 = 0) = \sum_{x_{\mathfrak{i}-1}} \Pr(X_{\mathfrak{i}} = 0 | X_{\mathfrak{i}-1} = x_{\mathfrak{i}-1}) \Pr(X_{\mathfrak{i}-1} = x_{\mathfrak{i}-1} | X_0 = 0)$$

- Start with $Pr(X_1 = 0 | X_0 = 0)$
- Get $Pr(X_1 = 1 | X_0 = 0)$
- Use these in formula with i=2
- Get $Pr(X_2 = 0 | X_0 = 0)$
- Get $Pr(X_2 = 1 | X_0 = 0)$
- Use these in formula with $\mathfrak{i}=3$
- Get $Pr(X_3 = 0 | X_0 = 0)$
- : : : :

Matrix Form

It is much easier to do this calculation in matrix form (especially when X is not binary). Let P be the transition matrix

$$\begin{array}{c|cccc} & X_i = 0 & X_i = 1 \\ \hline X_{i-1} = 0 & \text{Pr}(X_i = 0|X_{i-1} = 0) & \text{Pr}(X_i = 1|X_{i-1} = 0) \\ X_{i-1} = 1 & \text{Pr}(X_i = 0|X_{i-1} = 1) & \text{Pr}(X_i = 1|X_{i-1} = 1) \end{array}$$

Matrix Form

In our example:

Matrix Form

Let π_i be a 1×2 row vector which denotes the probabilities of each player winning Game i conditional on the initial Game

$$\pi_i = (\Pr(X_i = 0|X_0), \Pr(X_i = 1|X_0))$$
 (13)

In our example if $X_0 = 0$

$$\pi_1 = (0.8, 0.2) \tag{14}$$

In our example if $X_0 = 1$

$$\pi_1 = (0.3, 0.7) \tag{15}$$

Recursion in Matrix form

• The recursion formula is

$$\pi_{i} = \pi_{i-1} P \tag{16}$$

Therefore

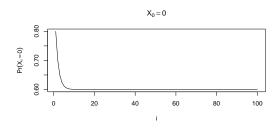
$$\pi_{n} = \pi_{1} P \times P \times \ldots \times P \tag{17}$$

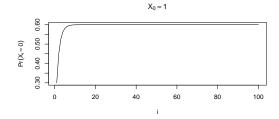
- Now code this up in R.
- What is $Pr(X_n = 0|X_0 = 0)$ when
 - n = 3
 - n = 5
 - n = 100?
- Do the same when $X_0 = 1$

Convergence?

- For n = 3 and n = 5, the starting point made a big difference.
- For n = 100 it did not make a big difference.
- Could this Markov chain be converging to something?
- Now write code to keep the values of π_i for i = 1, 2, ..., 100.
- Then plot the values of π_{i1} against i

Convergence





More Questions

- What is $Pr(X_{100} = 0|X_0 = 0)$?
- What is $Pr(X_{100} = 0 | X_0 = 1)$?
- What is $Pr(X_{1000} = 0|X_0 = 0)$?
- What is $Pr(X_{1000} = 0 | X_0 = 1)$?
- The answer to all of these is 0.6.
- The X do not converge. They keep changing from 0 to 1. The Markov chain however converges to a **stationary distribution**.

Simulation with a Markov chain

- Go back to your code for generating a Markov chain and generate a chain with $n=110000\,$
- ullet Exclude the first 10000 values of X_i and keep the remaining 100000 values.
- How many $X_i = 0$? How many $X_i = 1$
- We have discovered a new way to simulate from a distribution with $\Pr(X_i=0)=0.6$ and $\Pr(X_i=1)=0.4$

Markov Chains

 Sometimes two different Markov chains converge to the same stationary distribution. See what happens when

$$P = \begin{pmatrix} 0.9 & 0.1 \\ 0.15 & 0.85 \end{pmatrix}$$
 (18)

- Sometimes Markov chains do not converge to a stationary distribution at all.
- Some Markov chains can get stuck in an **absorbing state**. For example what would the simple example look like if $Pr(X_{i+1} = 0|X_i = 0) = 1$?
- Markov chains can be defined on continuous support as well, $X_{\rm i}$ can be continuous.

Some important points

- This is a very complicated way to generate from a simple distribution.
- For the binary example the direct method would be better.
- However for other examples, either the direct method or accept/reject algorithm do not work.
- In these cases we can construct a Markov chain that has a stationary distribution that is our target distribution.
- All we need is the kernel of the density function, and an algorithm called the Metropolis Algorithm

Normalizing Constant and Kernel

What are the normalizing constant and kernel of the Beta density?

$$\mathsf{Beta}(x; a, b) = \frac{\Gamma(a+b)}{(\Gamma(a)\Gamma(b))} x^{a-1} (1-x)^{b-1} \tag{19}$$

The Metropolis algorithm

- The Metropolis algorithm was developed in a 1953 paper by Metropolis, Rosenbluth, Rosenbluth, Teller and Teller.
- The aim is to simulate $x \sim p(x)$ where p(x) is called the **target density**.
- We will need a **proposal density** $q(x^{[old]} \rightarrow x^{[new]})$
- For example one choice of q is

$$x^{[new]} \sim N(x^{[old]}, 1)$$
 (20)

This is called a Random Walk proposal

Symmetric proposal

 An important property of q in the Metropolis algorithm is symmetry of the proposal

$$q(x^{[old]} \to x^{[new]}) = q(x^{[new]} \to x^{[old]}) \tag{21}$$

- Later we will not need this assumption
- Can you confirm this is true for $x^{[new]} \sim N(x^{[old]}, 1)$?
- Can you simulate from this random walk (use $x_0 = 0$ as a starting value)?

Proof of symmetry of random walk

The proposal

$$q(x^{[old]} \to x^{[new]}) = (2\pi)^{-1/2} \exp\left\{-\frac{1}{2} \left(x^{[new]} - x^{[old]}\right)^2\right\}$$
(22)
$$= (2\pi)^{-1/2} \exp\left\{-\frac{1}{2} \left[-1 \left(x^{[new]} - x^{[old]}\right)\right]^2\right\}$$
(23)

$$= (2\pi)^{-1/2} \exp\left\{-\frac{1}{2} \left(x^{[\text{old}]} - x^{[\text{new}]}\right)^2\right\}$$
 (24)

$$= q(x^{[new]} \to x^{[old]}) \tag{25}$$

Accept and reject

- By itself the random walk will not converge to anything.
- To make sure this Markov chain converges to our target, we need to include the following.
- At step i+1 set $x^{[old]}=x^{[i]}$.
- Generate $x^{[new]} \sim N(x^{[old]}, 1)$ and compute

$$\alpha = \min\left(1, \frac{p(x^{\lceil new \rceil})}{p(x^{\lceil old \rceil})}\right)$$
 (26)

- Then
 - Set $x^{[i+1]}$ to $x^{[new]}$ with probability α (accept)
 - Set $x^{[i+1]}$ to $x^{[old]}$ with probability $1-\alpha$ (reject)

Code it up

- Use the Metropolis algorithm with a random walk proposal to simulate a sample from the standard t distribution with 5 df.
- The target density is

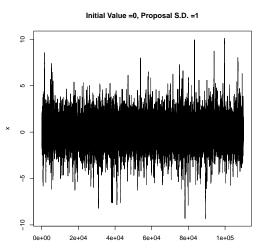
$$p(x) = \left[1 + \frac{x^2}{5}\right]^{-3} \tag{27}$$

- Simulate a Markov chain with 110000 iterates using the random walk as a proposal.
- The first 10000 iterates are the burn-in and will be left out because the Markov chain may not have converged yet.
- Use $x_0 = 0$ as a starting value

Some diagnostics - Convergence

- There a few diagnostics we can use to investigate the behaviour of the chain
- One is a trace plot (including burn in), which is simply a line plot of the iterates.
- Plot this for your Markov chain
- Another diagnostic is the Geweke diagnostic which can be found in the R package coda.
- The Geweke diagnostic tests the equality of the means of two different parts of the chain (excluding burn-in). The test statistic has a standard normal distribution.
- · Rejecting this test is evidence that the chain has not converged

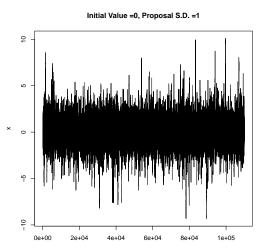
Trace Plot



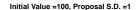
The effect of starting value

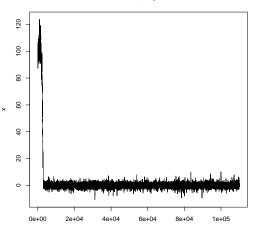
- Now rerun the code with a starting value of $X_0 = 100$
- Does the chain still converge?
- Does it converge quicker or slower?

Trace Plot



Trace Plot

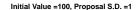


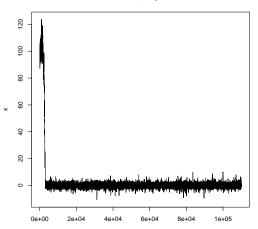


The effect of proposal variance

- Keep the starting value of $X_0 = 100$
- No change the standard deviation of the proposal to 3.
- Does the chain still converge?
- Does it converge quicker or slower?

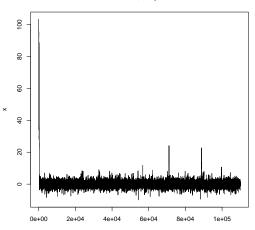
Trace Plot





Trace Plot



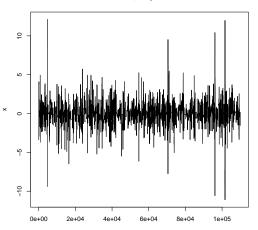


Huge proposal variance

- Maybe you think the best strategy is to choose a huge standard deviation.
- Try to use a proposal standard deviation of 100. Plot a trace plot of the chain.
- The plot is rejecting many iterates. This must be inefficient
- Change your code to compute the percentage of times a new iterate is accepted (excluding burn in).
- Use x_0 = as an initial value. What is the acceptance rate when the proposal standard deviation is 1? What is the acceptance rate when the proposal standard deviation is 100?

Trace Plot



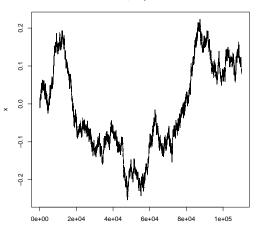


Acceptance Rate

- If the proposal variance is too high
 - Values will be proposed that are too far into the tails of the stationary distribution
 - The Metropolis algorithm will mostly reject these values.
 - The sample will still come from the correct target distribution but this is a very inefficient way to sample.
- What happens if a very small proposal variance is used.
- Try a proposal variance of 0.001. What is the acceptance rate?

Trace Plot





Acceptance Rate

- The acceptance rate is almost 1.
- However is this a good proposal?
- The jumps made by this proposal are too small, and do not sample enough iterates from the tails of the distribution.
- If it runs long enough the Markov chain will provide a sample from the target distribution. However, it is very inefficient.

Random Walk proposal

- For a random walk proposal it is not good to have an acceptance rate that is too high or too low.
- What exactly is too high and too low?
- It depends on many things including the target and proposal.
- A rough rule is to aim for an acceptance rate between 20% and 70%
- If your acceptance rate is outside this range the proposal variance can be doubled or halved
- There are better (but more complicated) ways to do this.

Monte Carlo Error

- Now that there is a sample. $X^{[1]}, X^{[2]}, \ldots, X^{[M]} \sim p(x)$. What can it be used for?
- We can estimate the expected value E(X)
- This can be done by taking:

$$E(X) \approx \frac{1}{M} \sum_{i=1}^{M} X^{[i]}$$

- Note we use \approx instead of =. There is some error since we are estimating E(X) based on a sample.
- Luckily we can make this smaller by generating a bigger sample.
- We call this Monte Carlo error.

Measuring Monte Carlo Error

• One way to measure Monte Carlo Error is the variance of the sample mean.

$$\begin{aligned} \text{Var}\left(\frac{1}{M}\sum_{i=1}^{M}X^{[i]}\right) &= \frac{1}{M^2}\text{Var}\left(\sum_{i=1}^{M}X^{[i]}\right) \\ &= \frac{1}{M^2}\sum_{i=1}^{M}\text{Var}(X^{[i]}) \\ &= \frac{\text{Var}(X)}{M} \end{aligned}$$

A sample from a Markov chain is correlated

Measuring Monte Carlo Error

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A sample from a Markov chain is correlated

Measuring Monte Carlo Error

• One way to measure Monte Carlo Error is the variance of the sample mean.

$$\begin{split} \text{Var}\left(\frac{1}{M}\sum_{i=1}^{M}X^{[i]}\right) &= \frac{1}{M^2}\text{Var}\left(\sum_{i=1}^{M}X^{[i]}\right) \\ &= \frac{1}{M^2}\sum_{i=1}^{M}\text{Var}(X^{[i]}) + \frac{2}{M^2}\sum_{i=1}^{M}\sum_{j>i}\text{cov}(X^{[i]},X^{[j]}) \\ &= \frac{\text{Var}(X)}{M} + \frac{2}{M^2}\sum_{i=1}^{M}\sum_{j>i}\text{cov}(X^{[i]},X^{[j]}) \end{split}$$

• A sample from a Markov chain is correlated

Monte Carlo efficiency

- It is better to have lower correlation in the Markov chain.
- The efficiency of the chain can be measured using the effective sample size.
- The effective sample size can be computed using the function *effectiveSize* in the R Package coda.
- Obtain an effective sample size for your sample (excluding burn in) where
 - Proposal S.D. =1
 - Proposal S.D. =5
- My answers were about 6000 and 18000 and yours should be close to that

Interpret Effective Sample Size

- What does it mean to say a Monte Carlo with a sample size of 100000 has an **effective sample size (ESS)** of just 6000?
- The sampling error of a correlated sample of 100000 is equal to the sampling error of an *independent sample* of 6000.
- Mathematically

$$\mathsf{Var}\left(\frac{1}{M}\sum_{\mathfrak{i}=1}^{M}X^{[\mathfrak{i}]}\right) = \frac{\mathsf{Var}(X)}{M} + \frac{2}{M^2}\sum_{\mathfrak{i}=1}^{M}\sum_{\mathfrak{j}>\mathfrak{i}}^{M}\mathsf{cov}(X^{[\mathfrak{i}]},X^{[\mathfrak{j}]}) = \frac{\mathsf{Var}(X)}{M_{eff}}$$

 It is a useful diagnostic for comparing two different proposal variances. A higher ESS implies a more efficient scheme.

Non-Symmetric proposal

- In 1970, Hastings proposed an extension to the Metropolis Hastings algorithm.
- This allows for the case when

$$q(x^{[old]} \to x^{[new]}) \neq q(x^{[new]} \to x^{[old]})$$
(28)

The only thing that changes is the acceptance probability

$$\alpha = \min\left(1, \frac{p(x^{[new]})q(x^{[new]} \to x^{[old]})}{p(x^{[old]})q(x^{[old]} \to x^{[new]})}\right)$$
(29)

• This is called the Metropolis-Hastings algorithm

An interesting proposal

• Suppose we use the proposal:

$$x^{\text{new}} \sim N(0, \sqrt{(5/3)}) \tag{30}$$

- What is $q(x^{[old]} \rightarrow x^{[new]})$?
- It is $q(x^{[new]})$ where q(.) is the density of a $N(0,\sqrt{(5/3)})$.
- Is this symmetric?
- No, since generally $q(x^{[new]}) \neq q(x^{[old]})$

Metropolis Hastings

- Code this where p(.) is the standard t density with 5 d.f, and q(.) is normal with mean 0 and standard deviation 5/3.
- Inside a loop
 - Generate $\chi^{[new]} \sim N(0, \sqrt{(5/3)})$
 - Set $x^{old} = x^{[i]}$ and compute

$$\alpha = \min\left(1, \frac{p(x^{[\text{new}]})q(x^{[\text{old}]})}{p(x^{[\text{old}]})q(x^{[\text{new}]})}\right)$$
(31)

- Set $x^{[i+1]}$ to $x^{[new]}$ with probability α (accept)
- Set $x^{[i+1]}$ to $x^{[old]}$ with probability $1-\alpha$ (reject)
- Try it

Comparison

- The Effective Sample Size of this proposal is about 43000 much higher than the best random walk proposal.
- Why does it work so well?
- The standard t distribution with 5 df has a mean of 0 and a standard deviation of $\sqrt{(5/3)}$
- So the $N(0, \sqrt{(5/3)})$ is a good approximation to the standard student t with 5 df.

Laplace Approximation

Using a Taylor expansion of lnp(x) around the point a

$$lnp(x) \approx lnp(\alpha) + \left. \frac{\partial lnp(x)}{\partial x} \right|_{x=\alpha} (x-\alpha) + \frac{1}{2} \left. \frac{\partial^2 lnp(x)}{\partial x^2} \right|_{x=\alpha} (x-\alpha)^2$$

Let α be the point that maximises lnp(x) and let

$$b = -\left(\frac{\partial^2 \ln p(x)}{\partial x^2}\Big|_{x=a}\right)^{-1}$$
 (32)

The approximation is

$$lnp(x) \approx lnp(a) - \frac{1}{2b}(x - a)^2$$

Taking exponential of both sides

$$p(x) \approx k \times exp\left[-\frac{(x-a)^2}{2b}\right]$$

Any distribution can be approximated by a normal distribution with mean α and variance b where α and b values can be found numerically if needed.

Exercise: Generating from skew normal

• The density of the skew normal is

$$p(x) = 2\phi(x)\Phi(\delta x) \tag{33}$$

where $\phi(x)$ is the density of the standard normal $\Phi(x)$ is the distribution of the standard normal.

- Using a combination of *optim*, *dnorm* and *pnorm* find the Laplace approximation of the skew normal when $\delta=3$
- Use it to generate a sample from the skew normal distribution using the Metropolis Hastings algorithm.

Indirect method v Metropolis Hastings

- Some similarities are:
 - Both require a proposal
 - Both are more efficient when the proposal is a good approximation to the target.
 - Both involve some form of accepting/rejecting
- Some differences are:
 - Indirect method produces an independent sample, MH samples are correlated.
 - Indirect method requires p(x)/q(x) to be finite for all x.
 - MH works better when x is a (high-dimensional vector).
- Why?

Multiple variables

- Suppose we now want to sample from a bivariate distribution p(x, z)
- The ideas involved in this section work for more than two variables.
- It is possible to do a 2-dimensional random walk proposal. However as the number of variables goes up the acceptance rate becomes lower.
- Also the Laplace approximation does not work as well in high dimensions.
- Indirect methods of simulation suffer from the same problem.
- We need a way to break the problem down.

Method of composition

- Markov chain methods, allow us to break multivariate distributions down.
- If it is easy to generate from p(x) then the best way is **Method of composition**. Generate
 - $x^{[i]} \sim p(x)$
 - $z^{[i]} \sim p(z|x=x^{[i]})$
- Sometimes p(x) is difficult to get

Gibbs Sampler

- If it is easy to simulate from the conditional distribution f(x|z) then that can be used as a proposal
- What is the acceptance ratio?

$$\begin{split} \alpha &= \left(1, \frac{p(x^{\text{new}}, z)p(x^{\text{old}}|z)}{p(x^{\text{old}}, z)p(x^{\text{new}}|z)}\right) \\ &= \left(1, \frac{p(x^{\text{new}}|z)p(z)p(x^{\text{old}}|z)}{p(x^{\text{old}}|z)p(z)p(x^{\text{new}}|z)}\right) \\ &= 1 \end{split}$$

Gibbs Sampler

- This gives the Gibbs Sampler
 - Generate $x^{[i+1]} \sim p(x^{[i+1]}|z^{[i]})$
 - Generate $z^{[i+1]} \sim p(z^{[i+1]}|x^{[i+1]})$
 - Repeat
- x and z can be swapped around.
- It works for more than two variables.
- Always make sure the conditioning variables are at the current state.

Metropolis within Gibbs

- Even if the individual conditional distributions are not easy to simulate from, Metropolis Hastings can be used *within* each Gibbs step.
- This works very well because it breaks down a multivariate problem into smaller univariate problems.
- We will practice some of these algorithms in the context of Bayesian Inference

Summary

- You should be familiar with a Markov chain
- You should understand this can have a stationary distribution
- You should have a basic understanding of the Metropolis Hastings and the special cases
 - Random Walk Metropolis
 - Laplace approximation
 - Gibbs Sampler