Bayesian Computation, Part 1

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Goal in any Bayesian Analysis

- Let X be some K dimensional array of random variables
- In Bayesian Learning we ultimately seek the joint distribution of X

$$\pi(X)$$

- From this we can derive other quantities of interest, e.g.,

$$\mathrm{E}[X] \equiv \int X \ \pi(X) \ dX$$

$$\Pr(X < c) = F(c) \equiv \int_{-\infty}^{c} \pi(X) dX,$$

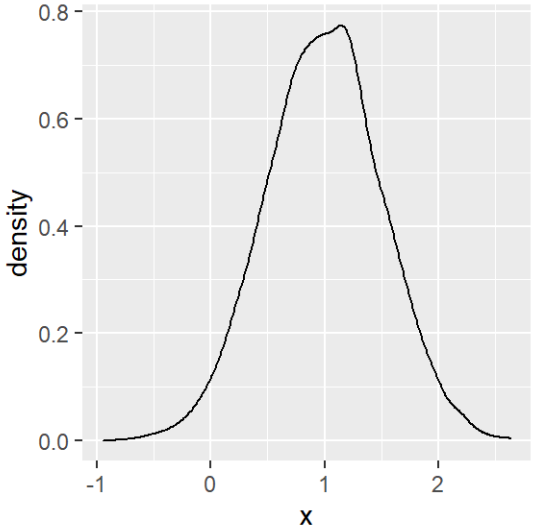
$$q = F^{-1}(p)$$

- These calculations can only be done analytically for the simplest models

Simulation

- One way to learn about a distribution is to analyze random draws from it!

```
## learning about a gaussian

library(tidyverse)

mu <- 1.0
sigma <- 0.5
nSim <- 10000
df <- data.frame(x = rnorm(n = nSim,
                           mean = mu,
                           sd = sigma))

e_x <- mean(df$x)
q_x <- quantile(df$x,probs=0.25)

pl <- df %>%
  ggplot(aes(x = x)) + geom_density()
```



- Simulated mean = 0.99418 (correct answer = 1)
- Simulated 25% quantile = 0.655 (correct answer = 0.663)

Easy to Sample From Distributions

- Normal and multivariate normal distribution
- t distribution (and Cauchy distribution)
- Gamma distribution (including exponential and chi-square distribution)
- F distribution
- Beta and Dirichlet distribution
- Poisson distribution
- Binomial distribution
- Negative Binomial distribution (and geometric distribution)
- Multinomial distribution

Simulation from Any Distribution

- Can we get direct independent draws from any probability distribution $\pi(X)$?
- No! Most joint posterior distributions derived from a Bayesian model do not have a known form that we can sample from directly
- Rather than sample directly from posteriors, we will use algorithms that will generate a stream of pseudo-random numbers which will converge to draws from the target distribution (the posterior)
- Specifically, almost all algorithms used in Bayesian computation are based on sampling from a carefully constructed continuous state Markov chain. "Carefully" constructed here means constructed so that the stationary distribution of the Markov chain is the posterior distribution from our Bayesian model. These are Markov Chain Monte Carlo (MCMC) algorithms

Time series model but time has no meaning.

- So we give up on getting direct independent draws from $\pi(X)$ - instead we will look for ways of generating a sequence of dependent draws $\{\tilde{X}_s\}_{s=1}^{S}$ which converges to draws from $\pi(X)$ as S gets large

Each iteration of loop will be a step in Markov chain. 收敛到正确的分布上来

- To understand how this works we first need a basic understand of Markov chains

Continous State Markov Chains

Time series model,

Time steps iteration
Time 1 Time 2 ..

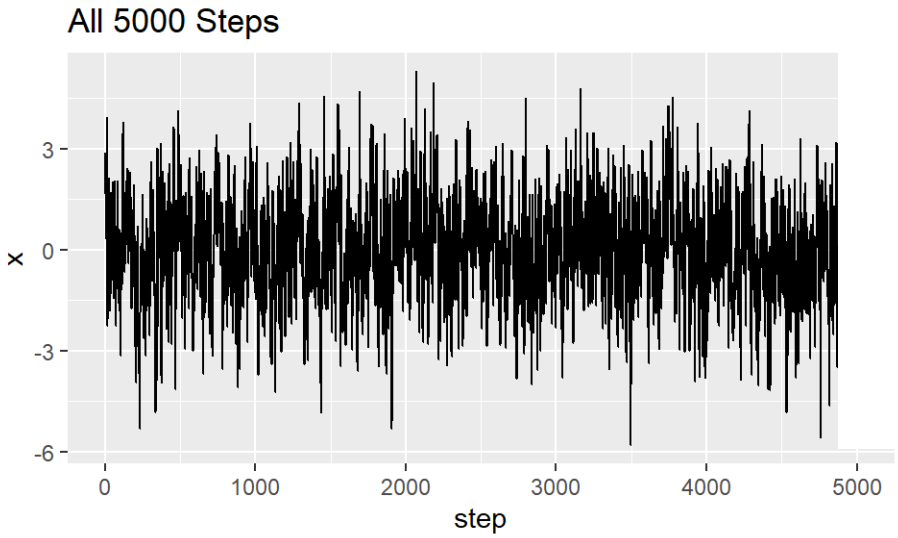
- We will use Discrete Time Continuous State Markov Chains
- The sequence $X_1, X_2, \ldots$ is a Markov chain if the distribution of X_t conditional $X_1, \ldots, X_{t-1}$ only depends on X_{t-1}: model for the evaluation of array

first order MC $$p(X_t|X_{t-1}, \ldots, X_1) = p(X_t|X_{t-1})$$ only depend on the most recent state

- The distribution on the right hand side is call the transition distribution
- Assuming we can easily sample from the transition distribution, then we can generate a realization of the Markov chain as
  - Start with a fixed X_0
  - Then sample X_1 as $X_1|X_0 \sim p(X_1|X_0)$
  - Sample X_2 as $X_2|X_1 \sim p(X_2|X_1)$
  - Sample X_3 as...

Example

$$X_t = \rho X_{t-1} + \varepsilon_t, \qquad |\rho| < 1$$
$$\varepsilon_t | \sigma \sim \mathrm{N}(0, \sigma^2)$$




```
rho <- 0.75
sigma <- 1.0

nSim <- 5000
eps <- rnorm(nSim, mean = 0, sd = sigma)

# initialize array and set beginning
df <- data.frame(x = array(0,nSim))
df$step <- 1

df$x[1] <- 2.5

for (t in 2:nSim){
  df$x[t] = rho*df$x[t-1] + eps[t]
  df$step[t] <- t
}
```

Stationary distribution

- The stationary distribution π of a Markov Chain with transition density $p(X|Z)$ is

$$\pi(X) = \int p(X|Z)\pi(Z)dZ$$

- Think of this as the point where the distribution underlying the Markov chain in no longer evolving - it has converged to a stationary distribution
- "Well behaved" Markov chains always converge to their stationary distribution. "Well behaved" has a specific mathematical definition. We will not go into these details here (see Chapter 11 of the Bayesian Data Analysis text book)
- In Bayesian computation we construct the transition distribution $p(X|Z)$ such that
  1. We can easily sample from $p(X|Z)$ and
  2. The implied stationary distribution $\pi(X)$ is the posterior distribution for the Bayesian model

Example

- The stationary distribution for the example above is

$$\pi(X) = \mathrm{N}\left(0, \frac{\sigma^2}{1-\rho^2}\right)$$

- Check: The transition distribution $p(X|Z)$ is

$$X = \rho Z + \varepsilon,$$

  where $\varepsilon \sim \mathrm{N}(0, \sigma^2)$. We need to show that if $Z \sim \pi(Z)$ then $X \sim \pi(X)$.

- To show this we can use the fact that a linear function of a normal distribution is another normal distribution with mean $\mathrm{E}[\rho Z + \varepsilon] = 0$ and variance

$$\mathrm{V}[\rho Z + \varepsilon] = \rho^2 \mathrm{V}[Z] + \mathrm{V}[\epsilon] = \rho^2 \frac{\sigma^2}{1-\rho^2} + \sigma^2 = \frac{\sigma^2}{1-\rho^2}$$

Markov Chain Monte Carlo Algorithms

Metropolis Algorithm

THE JOURNAL OF CHEMICAL PHYSICS VOLUME 21, NUMBER 6 JUNE, 1953

Equation of State Calculations by Fast Computing Machines

NICHOLAS METROPOLIS, ARIANNA W. ROSENBLUTH, MARSHALL N. ROSENBLUTH, AND AUGUSTA H. TELLER,
Los Alamos Scientific Laboratory, Los Alamos, New Mexico

AND

EDWARD TELLER,* *Department of Physics, University of Chicago, Chicago, Illinois*

(Received March 6, 1953)

A general method, suitable for fast computing machines, for investigating such properties as equations of state for substances consisting of interacting individual molecules is described. The method consists of a modified Monte Carlo integration over configuration space. Results for the two-dimensional rigid-sphere system have been obtained on the Los Alamos MANIAC and are presented here. These results are compared to the free volume equation of state and to a four-term virial coefficient expansion.

Arianna W. Rosenbluth, September 15, 1927 - December 28, 2020

Metropolis Algorithm

- Let $\pi(X)$ be the target distribution we want to sample from and let $p(X^*|X)$ be a symmetric proposal distribution generating a proposed move X^* of the chain, conditional on the current state X (symmetric means $p(X^*|X) = p(X|X^*)$)
- The algorithm starts with a starting value X_0 and then generates $\{X_t\}_{t=1}^T$ as follows:

1. Conditional on the current state X_{t-1}, generate a proposed move X^* from the proposal distribution:

$$X^* \sim p(X^*|X_{t-1})$$

2. Calculate

$$r = \min\left\{\frac{\pi(X^*)}{\pi(X_{t-1})}, 1\right\}$$

3. Update the new state X_t as

$$X_t = \begin{cases} X^* & \text{with probability } r, \\ X_{t-1} & \text{with probability } 1-r \end{cases}$$

Example

- Suppose we had to sample from a mixture of two bivariate normal distributions
- For $x = (x_1, x_2)$, the target density is

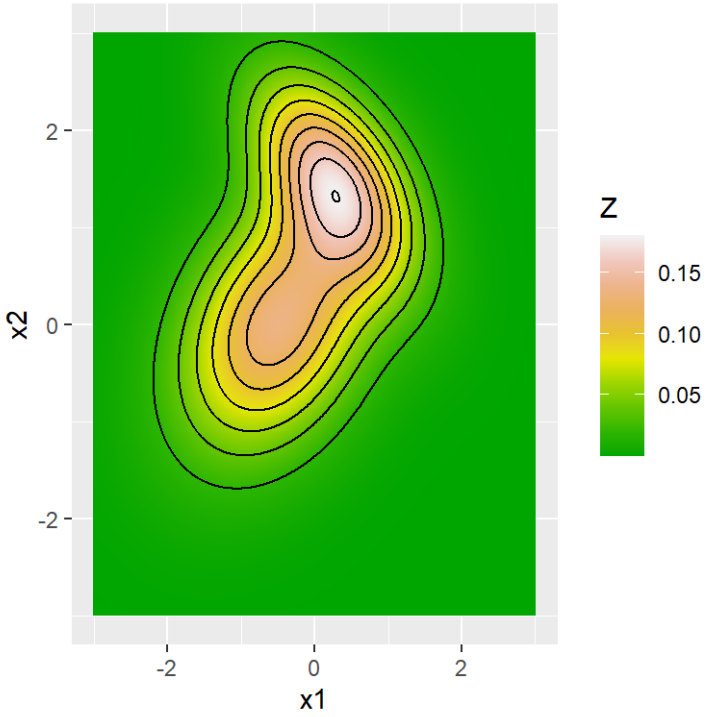
$$p(x) = \lambda \, \mathrm{N}(x|\mu_1, \Sigma_1) + (1 - \lambda) \, \mathrm{N}(x|\mu_2, \Sigma_2)$$

where $\mu_1 = (-0.5, 0.0)$, $\mu_2 = (0.25, 1.5)$ and

$$\Sigma_1 = \begin{bmatrix} 0.75 & 0.25 \\ 0.25 & 0.75 \end{bmatrix}, \quad \Sigma_2 = \begin{bmatrix} 0.5 & -0.25 \\ -0.25 & 0.5 \end{bmatrix}$$

and $\lambda = 0.6$

- Note: There are ways of sampling from this distribution directly, but let's imagine we don't know how to!



3D plot of target

Picking a Proposal Distribution

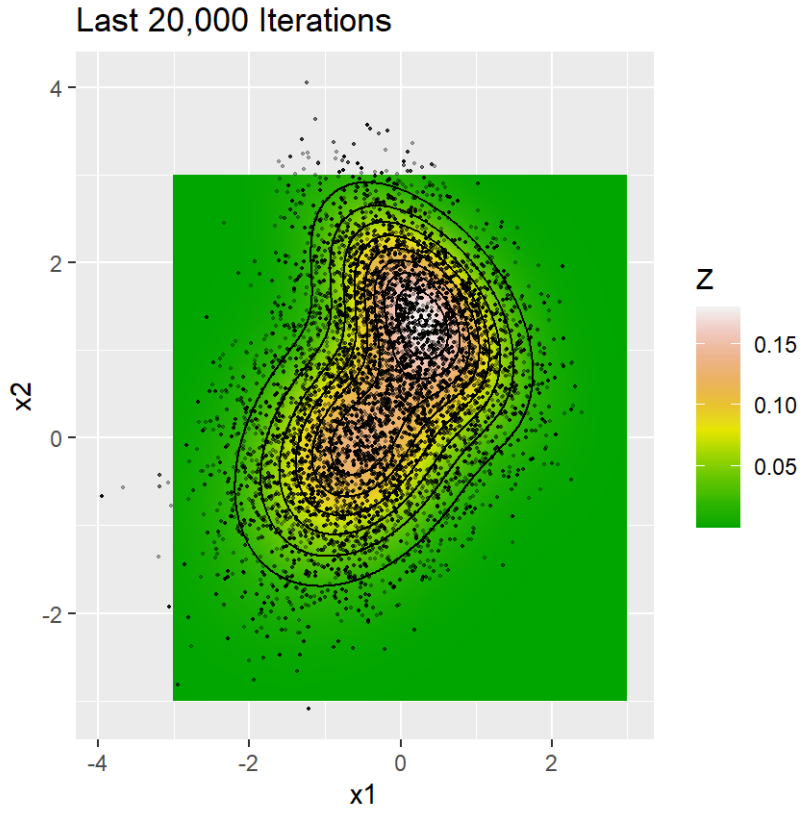
- The key ingredient in the Metropolis algorithm is picking the proposal distribution
- The proposal distribution should
  1. Be symmetric and
  2. Be easy to sample from and
  3. Generate draws that resemble the target distribution
- One class of proposal distributions that often work well is the random walk proposal:

$$X^* = X_{t-1} + \alpha\ \varepsilon$$

  where $\alpha > 0$ is a "jump" rate and usually $\epsilon \sim \mathrm{N}(0, I)$.
- α is chosen by experimentation to get a good compromise between a high acceptance rate and fast convergence to target distribution
  - If α is too big, most proposals will be rejected. If α is too small, the chain moves too slowly

Simulation Result

```r
alpha <- 1.0

nSim <- 10000
chain <- array(0,c(nSim,2))
acceptCount <- 0

for (i in 2:nSim){
  ## propose new move
  e <- rnorm(2, sd = alpha)
  x_star <- chain[i-1,] + e

  ## calculate accept rate
  dCurrent <- target(chain[i-1,])
  dNew <- target(x_star)

  r <- dNew/dCurrent

  if (runif(1) < r){
    chain[i,] <- x_star
    acceptCount <- acceptCount + 1
  } else {
    chain[i,] <- chain[i-1,]
  }
}
```



- Accept rate = 0.26

Sanity Check

- The target distribution has mean and covariance matrix

$$\mathrm{E}[X] = (-0.2, 0.6),$$
$$\mathrm{V}[X] = \begin{bmatrix} 0.79 & 0.32 \\ 0.32 & 1.19 \end{bmatrix}$$

- If our samples are from the correct distribution - and we have enough of them - then we should be able to get close to these values by simply looking at the sample average and covariance of the sampled values:

```
##         X1         X2
## -0.1969371  0.6223735
```

```
##           X1        X2
## X1 0.7452475 0.3110285
## X2 0.3110285 1.1878245
```

Metropolis Example: Logit Classifier

- Suppose we have classes $Y \in \{0, 1\}$ and features X and we assume

$$\Pr(Y = 1|X, \beta) = \frac{\exp\{\beta' X\}}{1 + \exp\{\beta' X\}}$$

- Normally we train this model by maximizing the log-likelihood function:

$$\log L(\beta) = \sum_{i=1}^{N} Y_i \log \Pr(Y_i = 1|X_i, \beta) + (1 - Y_i) \log \Big(1 - \Pr(Y_i = 1|X_i, \beta)\Big)$$

- If we specify a prior $\pi(\beta)$, then the log-posterior is

$$\log p(\beta) = \log L(\beta) + \log \pi(\beta)$$

- Let's try to train this model using the Metropolis algorithm with a random walk proposal distribution

Synthetic Data

- Generate 1,000 observations with

$$X_i = (1,\ x_{i2},\ x_{i3},\ x_{i4},\ x_{i5}),$$

  and $x_{ij} \sim \mathrm{N}(0, 1)$

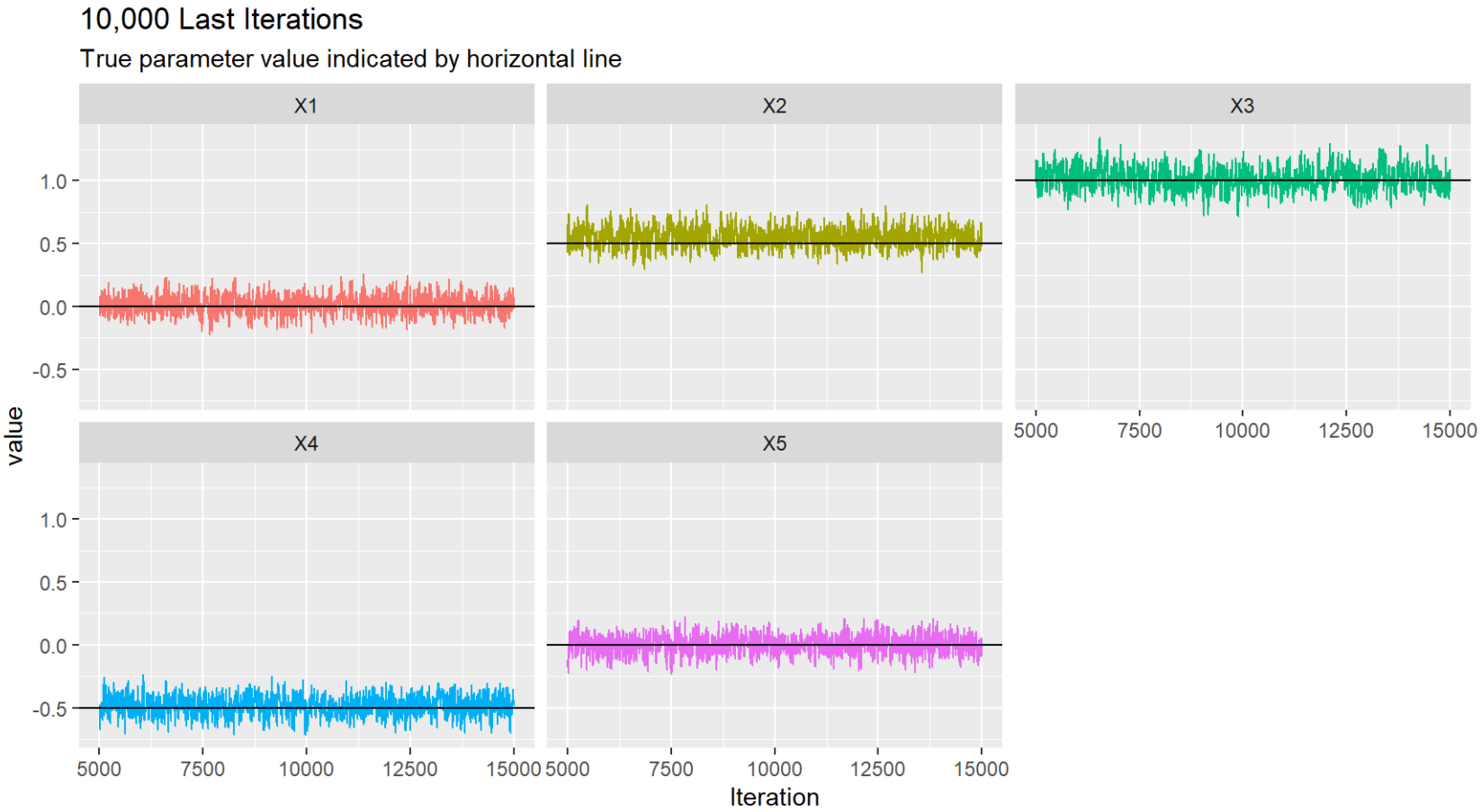
- The true β is

$$\beta = (0.0, 0.5, 1.0, -0.5, 0.0)$$

- We use a prior

$$\beta \sim \mathrm{N}(0, \tau^{-1} I_5)$$

Result


10,000 Last Iterations
True parameter value indicated by horizontal line
X1
X2
X3
X4
X5
value
1.0
0.5
0.0
-0.5
5000
7500
10000
12500
15000
Iteration

Metropolis-Hastings

- This is a generalization of the Metropolis algorithm that allows for non-symmetric proposal distributions
- All we need is to correct the acceptance probability by including the proposal:

$$r = \min \left\{ \frac{\pi(X^*)/p(X^*|X_{t-1})}{\pi(X_{t-1})/p(X_{t-1}|X^*)}, 1 \right\}$$

- Other than that everything else is the same

Problem with Metropolis

- The Metropolis (and Metropolis-Hastings) algorithm is a great general purpose algorithm
- There is one downside: In large dimensions it often runs into a big problem: Almost all proposals get rejected!
- The bigger the dimension of X is, the more likely it is that some elements of X are outside of the mass of $\pi(X)$ and therefore the entire X gets rejected
- This happens since the advantage of the Metropolis algorithm is also a disadvantage: The proposal distribution doesn't use any information about $\pi(X)$
- Thankfully, there is another general algorithm that we can rely on in large dimensions

Gibbs Sampling

IEEE TRANSACTIONS ON PATTERN ANALYSIS AND MACHINE INTELLIGENCE, VOL. PAMI-6, NO. 6, NOVEMBER 1984 721

Stochastic Relaxation, Gibbs Distributions, and the Bayesian Restoration of Images

STUART GEMAN AND DONALD GEMAN

Abstract—We make an analogy between images and statistical mechanics systems. Pixel gray levels and the presence and orientation of edges are viewed as states of atoms or molecules in a lattice-like physical system. The assignment of an energy function in the physical sys-

The essence of our approach to restoration is a stochastic relaxation algorithm which generates a sequence of images that converges in an appropriate sense to the MAP estimate. This sequence evolves by *local* (and potentially *parallel*) changes in

Gibbs Sampling

- The Gibbs sampler is based on a very basic observation: All information in a joint distribution $p(X_1, X_2)$ is contained in the two conditional distributions $p(X_1|X_2)$ and $p(X_2|X_1)$ (subject to some very mild assumptions)
- The Gibbs sampler is based on constructing a Markov chain where the transition distribution is made up of each of the conditional distributions:
- Start with $X_{2,0}$. Then sample $\{X_{1t}, X_{2t}\}_{t=1}^{T}$ as

$$\begin{aligned} X_{1t}|X_{2t-1} &\sim p(X_{1t}|X_{2t-1}), \\ X_{2t}|X_{1t} &\sim p(X_{2t}|X_{1t}), \end{aligned}$$

- Basic advantage: It is easier to sample from a series of conditional distributions than directly from the joint distribution

Gibbs Sampling

- You can run the Gibbs sampler on any number of partitions of the full variable X
- For example, dividing X into three arrays $X = (X_1, X_2, X_3)$, the Gibbs sampler is

$$\begin{aligned} X_{1t}|X_{2t-1}, X_{3t-1} &\sim p(X_{1t}|X_{2t-1}, X_{3t-1}), \\ X_{2t}|X_{1t}, X_{3t-1} &\sim p(X_{2t}|X_{1t}, X_{3t-1}), \\ X_{3t}|X_{1t}, X_{2t} &\sim p(X_{3t}|X_{1t}, X_{2t}) \end{aligned}$$

- Now - let's look at some examples of how to derive the required conditional distributions

Example 1

- Consider the simple normal distribution model:

$$X_i|\mu,\tau \sim \mathrm{N}(\mu,\tau^{-1}), \qquad i = 1,\ldots,N$$

  where we use a normal prior for μ and a gamma distribution for τ (the precision = 1/variance):

$$\mu \sim \mathrm{N}(\mu_0,\tau_0^{-1}),$$
$$\tau \sim \mathrm{G}(a_0,b_0)$$

- We need to find the conditional distributions $p(\mu|\tau,X)$ and $p(\tau|\mu,X)$
- Note that we have already derived $p(\mu|\tau,X)$ - we did this in week 1, example III (see slide 29):

$$p(\mu|\tau,X) = \mathrm{N}(m,c^{-1}), \quad c \equiv \tau N + \tau_0, \quad m \equiv \frac{\tau\sum_i X_i + \tau_0\mu_0}{c}$$

Gamma Distribution

- The Gamma distribution is a distribution on the positive real axis:

$$\mathrm{G}(\tau|a_0, b_0) = \frac{{b_0}^{a_0}}{\Gamma(a_0)}\tau^{a_0-1}\exp(-b_0\tau),$$

  with the properties

$$\mathrm{E}[\tau] = \frac{a_0}{b_0},$$
$$\mathrm{V}[\tau] = \frac{a_0}{b_0^2}$$

- This allows us to express a wide range of beliefs about τ

- Next we need the other conditional $p(\tau|\mu, X)$
- Again from Week 1, slide 29 we have the likelihood function

$$p(X_1, \ldots, X_N|\mu, \tau) = \left(\frac{1}{\sqrt{2\pi}}\right)^N \tau^{N/2} \exp\left(-\frac{\tau}{2} ssq\right)$$

$ssq = \sum_{i=1}^{N}(X_i - \mu)^2$

- Therefore the conditional for τ is

$$\begin{aligned} p(\tau|\mu, X) &= p(X_1, \ldots, X_N|\mu, \tau) \times \mathrm{G}(\tau|a_0, b_0) \\ &= C \times \tau^{N/2} \exp\left(-\frac{\tau}{2} ssq\right) \times \tau^{a_0-1} \exp(-b_0\tau) \\ &= C \times \tau^{a_0+N/2-1} \exp\left\{-\tau(b_0 + \tfrac{1}{2} ssq)\right\} \end{aligned}$$

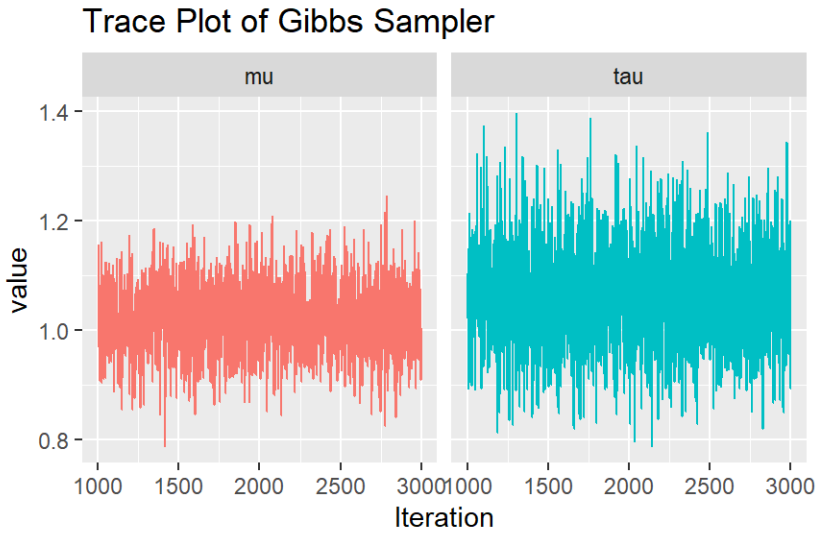
- We recognize this as another as another Gamma distribution: $\mathrm{G}(a_0 + N/2, b_0 + \frac{1}{2} ssq)$

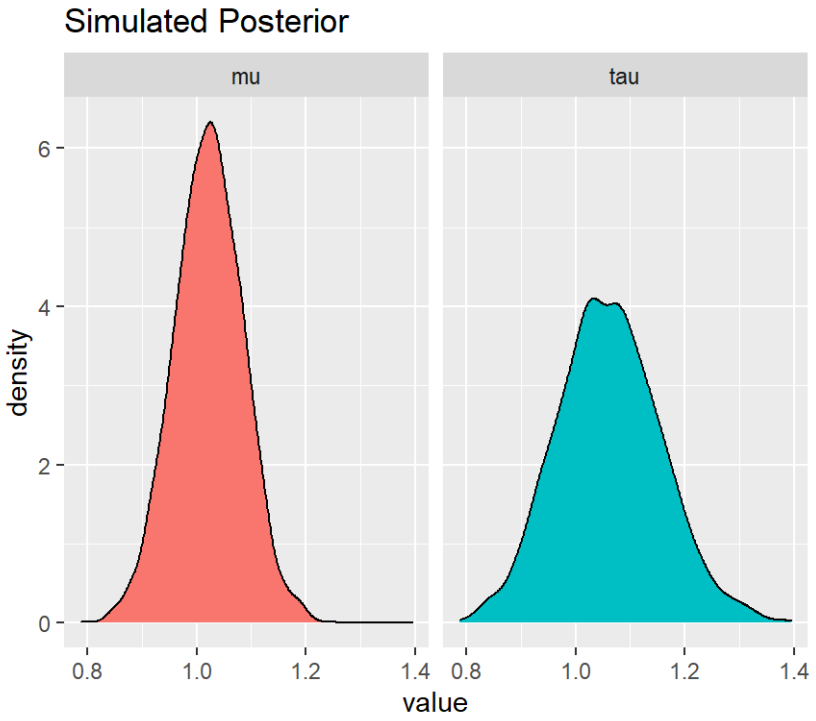
Gibbs Sampler

- We have derived our first Gibbs sampler which simply means repeatedly sampling from
  1. $\mu_t|\tau_{t-1} \sim \mathrm{N}\left(m(\tau_{t-1}), c(\tau_{t-1})^{-1}\right)$
  2. $\tau_t|\mu_t \sim \mathrm{G}\left(a_0 + N/2, b_0 + \frac{1}{2}ssq(\mu_t)\right)$
- This requires that we are able to sample from a Normal and Gamma distribution but that is easy

```
for (i in 2:nIter){
  ## mu|tau
  mu_var <- 1.0/(gibbsDF$tau[i-1]*N + tau0)
  mu_mean <- mu_var*(gibbsDF$tau[i-1]*sum_x + tau0*mu0)
  gibbsDF$mu[i] <- rnorm(1,mean = mu_mean, sd = sqrt(mu_var))

  ## tau|mu
  ag <- a0 + 0.5*N
  bg <- b0 + 0.5*sum((df$X - gibbsDF$mu[i])^2)
  gibbsDF$tau[i] <- rgamma(1,shape = ag, rate = bg)
}
```

Result






```
## # A tibble: 2 x 5
##   parameter  mean median  q2.5 q97.5
##   <chr>     <dbl>  <dbl> <dbl> <dbl>
## 1 mu         1.02   1.02 0.897  1.14
## 2 tau        1.06   1.06 0.888  1.26
```

Example 2: Uber Revisited

$$y_{ij}|\alpha_i, \sigma \sim \mathrm{N}(\alpha_i, \tau^{-1}), \qquad j = 1, \ldots, N_i; i = 1, \ldots, N,$$

with priors

$$\begin{aligned}
\alpha_i|\mu, \sigma_\alpha &\sim \mathrm{N}(\mu_\alpha, \tau_\alpha^{-1}), \\
\mu_\alpha &\sim \mathrm{N}(\mu_0, \tau_0^{-1}), \\
\tau &\sim \mathrm{G}(a_0, b_0), \\
\tau_\alpha &\sim \mathrm{G}(c_0, d_0),
\end{aligned}$$

Conditional Distributions

- We already know how to get the conditional for α_i and μ_α - this is exactly as above:

$$\alpha_i | Y, \mu_\alpha, \tau_\alpha, \tau \sim \mathrm{N}(m_i, c_i^{-1}),$$

  where $c_i = \tau N_i + \tau_\alpha$ and $m_i = c_i^{-1}(\tau \sum_{j=1}^{N_i} X_{ij} + \tau_\alpha \mu_\alpha)$

- For μ_α this gives us

$$\mu_\alpha|\alpha, \tau_\alpha \sim \mathrm{N}(m, c^{-1})$$

where $c = \tau_\alpha N + \tau_0$ and $m = c^{-1}(\tau_\alpha \sum_{i=1}^{N} \alpha_i + \mu_0 \tau_0)$

- For τ_α we can again follow the derivation in Example 1 to get

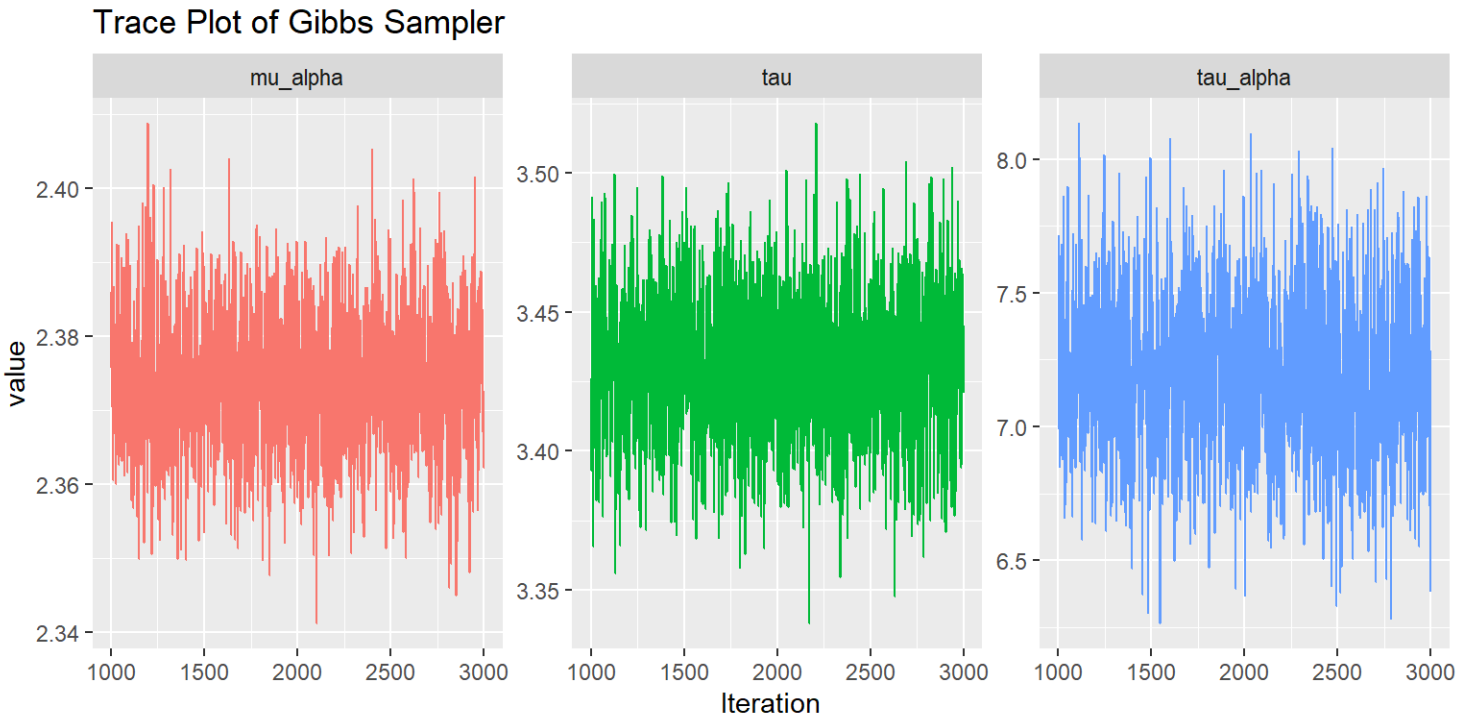
$$\tau_\alpha|\alpha, \mu_\alpha \sim \mathrm{G}\Big(c_0 + \tfrac{1}{2}N, d_0 + \tfrac{1}{2}\sum_{i=1}^{N}(\alpha_i - \mu_\alpha)^2\Big)$$

- Finally for τ we can follow a similar derivation across i and j to get

$$\tau|\alpha, Y \sim \mathrm{G}\Big(a_0 + \tfrac{1}{2}\sum_{i=1}^{N} N_i, b_0 + \tfrac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N_i}(Y_{ij} - \alpha_i)^2\Big)$$

Code

```
for (i in 2:nIter){
  ## alpha
  mu_var <- 1.0/(gibbs1$tau[i-1]*dfStats$n_i + gibbs1$tau_alpha[i-1])
  mu_mean <- mu_var*(gibbs1$tau[i-1]*dfStats$sumY +
                       gibbs1$tau_alpha[i-1]*gibbs1$mu_alpha[i-1])
  gibbs2[i,] <- mu_mean + sqrt(mu_var)*rnorm(nRiders)

  ## mu_alpha
  mu_var <- 1.0/(gibbs1$tau_alpha[i-1]*nRiders + tau0)
  mu_mean <- mu_var*(gibbs1$tau_alpha[i-1]*sum(gibbs2[i,]) + tau0*mu0)
  gibbs1$mu_alpha[i] <- rnorm(1,mean = mu_mean, sd = sqrt(mu_var))

  ## tau_alpha
  ag <- c0 + 0.5*nRiders
  bg <- d0 + 0.5*sum((gibbs2[i,] - gibbs1$mu_alpha[i])^2)
  gibbs1$tau_alpha[i] <- rgamma(1,shape = ag, rate = bg)

  ## tau
  ag <- c0 + 0.5*nTotal
  bg <- d0 + 0.5*( ssqAll + sum(dfStats$n_i*(gibbs2[i,]^2)) -
                     2.0*sum(gibbs2[i,]*dfStats$sumY))
  gibbs1$tau[i] <- rgamma(1,shape = ag, rate = bg)
}
```


Trace Plot of Gibbs Sampler
mu_alpha
tau
tau_alpha
value
Iteration
2.40
2.38
2.36
2.34
3.50
3.45
3.40
3.35
8.0
7.5
7.0
6.5
1000
1500
2000
2500
3000

Comparison to Stan Run (Week 2)

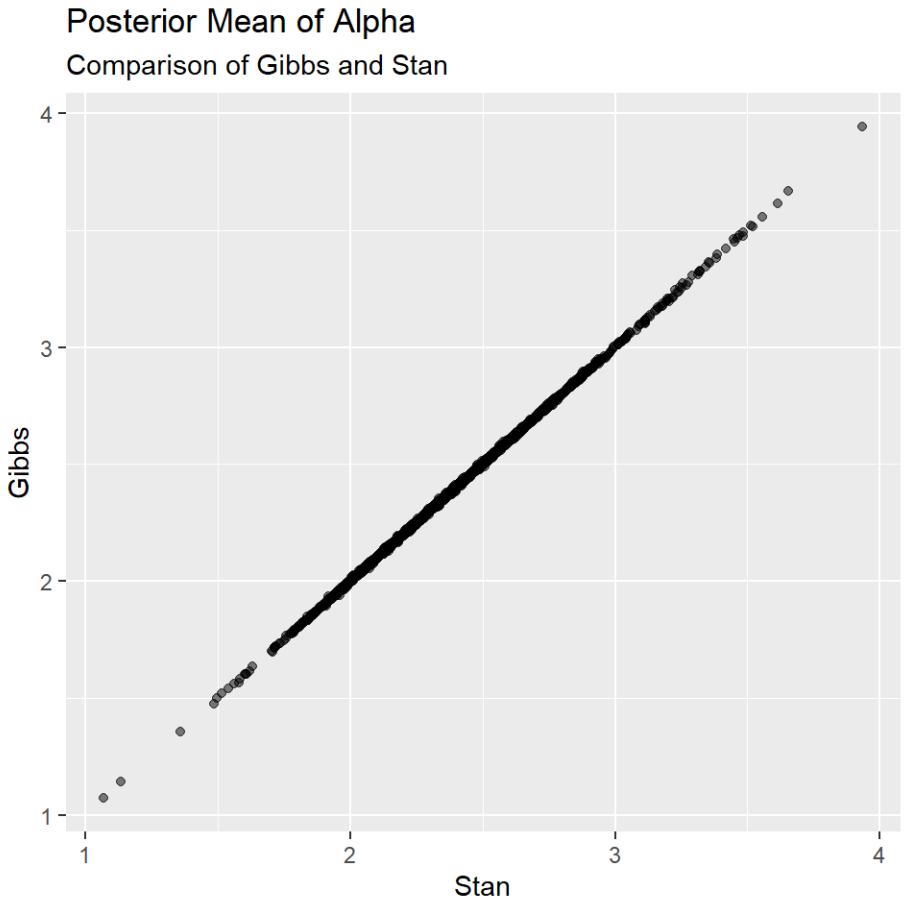
- Gibbs Summary:

```
## # A tibble: 3 x 5
##   parameter  mean median  q2.5 q97.5
##   <chr>     <dbl>  <dbl> <dbl> <dbl>
## 1 mu_alpha   2.37   2.37  2.36  2.39
## 2 tau        3.43   3.43  3.38  3.48
## 3 tau_alpha  7.21   7.21  6.64  7.79
```

- Stan Summary:

```
## # A tibble: 3 x 5
##   parameter  mean median  q2.5 q97.5
##   <chr>     <dbl>  <dbl> <dbl> <dbl>
## 1 mu_alpha   2.37   2.37  2.35  2.39
## 2 tau        3.43   3.43  3.38  3.48
## 3 tau_alpha  7.25   7.24  6.68  7.84
```

Comparison to Stan Run (Week 2)



HMC and Stan

- HMC = Hybrid Monte Carlo
- This is a version of Metropolis-Hastings where we use information about the gradient of the log-posterior to propose promising moves
- This often leads to algorithms with high acceptance rates and fast convergence
- Can be implemented manually or by using Stan
- Next module!