

Module 7: Introduction to Gibbs Sampling

Rebecca C. Steorts

Announcements

- ▶ Exam II will be Thursday October 29th (it will be open note, open book)
- ▶ No required class on November 3rd (Election day). I will post an ansyn. lecture for you to watch at your convenience so we don't get behind on material.
- ▶ There are more practice problems posted (and more coming).
- ▶ Thank you for all the feedback from the survey.
- ▶ If you are a student that needs an extra OH, please email me by tomorrow at 5 PM so I can organize this with three preferred times.
- ▶ Detailed takeways have been posted for each module (1-6) to help you prepare for exams.

Agenda

- ▶ Background knowledge (inverse CDF method)
- ▶ Gibbs sampling (two-stage sampler)
- ▶ Exponential example
- ▶ Normal example
- ▶ Pareto example
- ▶ Diagnostics

Background knowledge

The inverse CDF technique for generating a random sample uses the fact that a continuous CDF, F , is a one-to-one mapping of the domain of the CDF into the interval $(0, 1)$.

Lemma

If U is a uniform random variable on $(0, 1)$, then $X = F^{-1}(U)$ has the distribution F .

Formal Proof: <https://www.youtube.com/watch?v=irheiVXJRm8>

Gibbs sampler

- ▶ Suppose $p(x, y)$ is a p.d.f. or p.m.f. that is difficult to sample from directly.
- ▶ Suppose, though, that we *can* easily sample from the conditional distributions $p(x|y)$ and $p(y|x)$.
- ▶ The Gibbs sampler proceeds as follows:
 1. set x and y to some initial starting values
 2. then sample $x|y$, then sample $y|x$, then $x|y$, and so on.

Gibbs sampler

0. Set (x_0, y_0) to some starting value.
1. Sample $x_1 \sim p(x|y_0)$, that is, from the conditional distribution $X | Y = y_0$.

Current state: (x_1, y_0)

Sample $y_1 \sim p(y|x_1)$, that is, from the conditional distribution $Y | X = x_1$.

Current state: (x_1, y_1)

2. Sample $x_2 \sim p(x|y_1)$, that is, from the conditional distribution $X | Y = y_1$.

Current state: (x_2, y_1)

Sample $y_2 \sim p(y|x_2)$, that is, from the conditional distribution $Y | X = x_2$.

Current state: (x_2, y_2)

⋮

Repeat iterations 1 and 2, M times.

Gibbs sampler

This procedure defines a sequence of pairs of random variables

$$(X_0, Y_0), (X_1, Y_1), (X_2, Y_2), (X_3, Y_3), \dots$$

Markov chain and dependence

$$(X_0, Y_0), (X_1, Y_1), (X_2, Y_2), (X_3, Y_3), \dots$$

satisfies the property of being a Markov chain.

The conditional distribution of (X_{i+1}, Y_{i+1}) given all of the previous pairs depends only on (X_i, Y_i)

Example: The conditional distribution of (X_5, Y_5) given all of the previous pairs depends only on (X_4, Y_4)

$(X_0, Y_0), (X_1, Y_1), (X_2, Y_2), (X_3, Y_3), \dots$ are not iid samples (Think about why).

Ideal Properties of MCMC

- ▶ (x_0, y_0) chosen to be in a region of high probability under $p(x, y)$, but often this is not so easy.
- ▶ We run the chain for M iterations and discard the first B samples $(X_1, Y_1), \dots, (X_B, Y_B)$. This is called *burn-in*.
- ▶ Typically: if you run the chain long enough, the choice of B doesn't matter.
- ▶ Roughly speaking, the performance of an MCMC algorithm—that is, how quickly the sample averages $\frac{1}{N} \sum_{i=1}^N h(X_i, Y_i)$ converge—is referred to as the *mixing rate*.
- ▶ An algorithm with good performance is said to “have good mixing”, or “mix well”.

Exponential Example

Consider the following Exponential model for observation(s)
 $x = (x_1, \dots, x_n)$.¹:

$$p(x|a, b) = ab \exp(-abx)I(x > 0)$$

and suppose the prior is

$$p(a, b) = \exp(-a - b)I(a, b > 0).$$

You want to sample from the posterior $p(a, b|x)$.

¹Please note that in the attached data there are 40 observations, which can be found in data-exponential.csv.

Conditional distributions

$$\begin{aligned} p(\mathbf{x}|a, b) &= \prod_{i=1}^n p(x_i|a, b) \\ &= \prod_{i=1}^n ab \exp(-abx_i) \\ &= (ab)^n \exp\left(-ab \sum_{i=1}^n x_i\right). \end{aligned}$$

The function is symmetric for a and b , so we only need to derive $p(a|\mathbf{x}, b)$.

Conditional distributions

This conditional distribution satisfies

$$\begin{aligned} p(a|\mathbf{x}, b) &\propto_a p(a, b, \mathbf{x}) \\ &= p(\mathbf{x}|a, b)p(a, b) \\ &= \text{fill in full details for lab this week} \end{aligned}$$

Gibbs sampling code

```
knitr::opts_chunk$set(cache=TRUE)
library(MASS)
data <- read.csv("data-exponential.csv", header = FALSE)
```

Gibbs sampling code

```
#####  
# This function is a Gibbs sampler  
#  
# Args  
#   start.a: initial value for a  
#   start.b: initial value for b  
#   n.sims: number of iterations to run  
#   data: observed data, should be in a  
#         # data frame with one column  
#  
# Returns:  
#   A two column matrix with samples  
#     #   for a in first column and  
#   samples for b in second column  
#####
```

Gibbs sampling code

```
sampleGibbs <- function(start.a, start.b, n.sims, data){  
  # get sum, which is sufficient statistic  
  x <- sum(data)  
  # get n  
  n <- nrow(data)  
  # create empty matrix, allocate memory for efficiency  
  res <- matrix(NA, nrow = n.sims, ncol = 2)  
  res[1,] <- c(start.a, start.b)  
  for (i in 2:n.sims){  
    # sample the values  
    res[i,1] <- rgamma(1, shape = n+1,  
                      rate = res[i-1,2]*x+1)  
    res[i,2] <- rgamma(1, shape = n+1,  
                      rate = res[i,1]*x+1)  
  }  
  return(res)  
}
```

Gibbs sampler code

```
# run Gibbs sampler  
n.sims <- 10000  
# return the result (res)  
res <- sampleGibbs(.25,.25,n.sims,data)  
head(res)
```

```
##           [,1]      [,2]  
## [1,] 0.2500000 0.2500000  
## [2,] 1.6230745 0.3364386  
## [3,] 1.4990049 0.3614046  
## [4,] 1.1995143 0.6831900  
## [5,] 0.8522461 0.7157094  
## [6,] 0.5959641 0.6798289
```


Exponential Example

You will explore this problem more in lab this week and in your homework.

Toy Example

$$p(x, y) \propto e^{-xy} \mathbb{1}(x, y \in (0, c))$$

$$p(x|y) \underset{x}{\propto} p(x, y) \underset{x}{\propto} e^{-xy} \mathbb{1}(0 < x < c) \underset{x}{\propto} \text{Exp}(x|y) \mathbb{1}(x < c).^2$$

- ▶ $p(x|y)$ is a *truncated* version of the $\text{Exp}(y)$ distribution
- ▶ It is the same as taking $X \sim \text{Exp}(y)$ and conditioning on it being less than c , i.e., $X \mid X < c$.
- ▶ Let's refer to this as the $\text{TExp}(y, (0, c))$ distribution.

²Under \propto , we write the random variable (x) for clarity.

Toy Example

- ▶ The Gibbs sampling approach is to alternately sample from $p(x|y)$ and $p(y|x)$.
- ▶ Note $p(x, y)$ is symmetric with respect to x and y .
- ▶ Hence, only need to derive one of these and then we can get the other one by just swapping x and y .
- ▶ Let's look at $p(x|y)$.

Toy Example

An easy way to generate a sample from $Z \sim \text{TExp}(\theta, (0, c))$, is:

1. Sample $U \sim \text{Uniform}(0, F(c|\theta))$ where

$$F(x|\theta) = 1 - e^{-\theta x}$$

is the $\text{Exp}(\theta)$ c.d.f.

2. Set $Z = F^{-1}(U|\theta)$ where

$$F^{-1}(u|\theta) = -(1/\theta) \log(1 - u)$$

is the inverse c.d.f. for $u \in (0, 1)$.

There is an exercise on the next slide to prove step 2.

Toy Example

Practice Exercise: Verify that

$$F^{-1}(u|\theta) = -(1/\theta) \log(1 - u).$$

Solution:

To solve for F^{-1} , set $u = F(x)$ for $u \in (0, 1)$ and solve for x .

$$\begin{aligned} u &= 1 - e^{-\theta x} \implies \\ e^{-\theta x} &= 1 - u \implies \\ -\theta x &= \log(1 - u) \implies \\ x &= -\frac{1}{\theta} \log(1 - u). \end{aligned}$$

This proves that $F^{-1}(u|\theta) = -(1/\theta) \log(1 - u)$.

Toy example

Let's apply Gibbs sampling, denoting $S = (0, c)$.

0. Initialize $x_0, y_0 \in S$.
1. Sample $x_1 \sim \text{TExp}(y_0, S)$, then sample $y_1 \sim \text{TExp}(x_1, S)$.
2. Sample $x_2 \sim \text{TExp}(y_1, S)$, then sample $y_2 \sim \text{TExp}(x_2, S)$.
- \vdots
- N . Sample $x_N \sim \text{TExp}(y_{N-1}, S)$, sample $y_N \sim \text{TExp}(x_N, S)$.

Figure 1 demonstrates the algorithm, with $c = 2$ and initial point $(x_0, y_0) = (1, 1)$.

Toy example

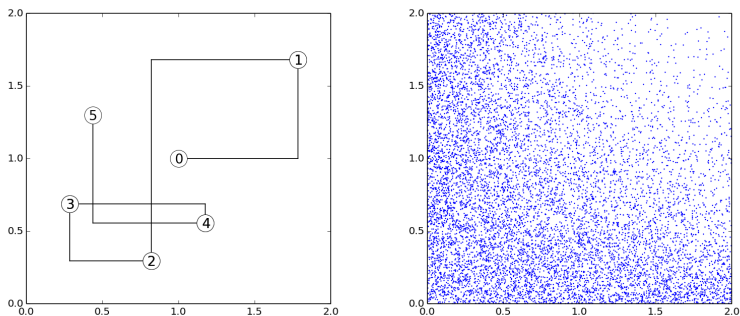


Figure 1: (Left) Schematic representation of the first 5 Gibbs sampling iterations/sweeps/scans. (Right) Scatterplot of samples from 10^4 Gibbs sampling iterations.

Example: Normal with semi-conjugate prior

Consider $X_1, \dots, X_n | \mu, \lambda \stackrel{iid}{\sim} \mathcal{N}(\mu, \lambda^{-1})$. Then independently consider

$$\mu \sim \mathcal{N}(\mu_0, \lambda_0^{-1})$$

$$\lambda \sim \text{Gamma}(a, b)$$

This is called a semi-conjugate situation, in the sense that the prior on μ is conjugate for each fixed value of λ , and the prior on λ is conjugate for each fixed value of μ .

For ease of notation, denote the observed data points by $x_{1:n}$.

How does one derive $p(\mu, \lambda \mid x_{1:n})$?

Example

We know that for the Normal–Normal model, we know that for any fixed value of λ ,

$$\boldsymbol{\mu}|\lambda, \mathbf{x}_{1:n} \sim \mathcal{N}(\mathbf{M}_\lambda, L_\lambda^{-1})$$

where

$$L_\lambda = \lambda_0 + n\lambda \quad \text{and} \quad \mathbf{M}_\lambda = \frac{\lambda_0 \boldsymbol{\mu}_0 + \lambda \sum_{i=1}^n \mathbf{x}_i}{\lambda_0 + n\lambda}.$$

For any fixed value of μ , it is straightforward to derive³ that

$$\lambda|\mu, \mathbf{x}_{1:n} \sim \text{Gamma}(A_\mu, B_\mu) \tag{1}$$

where $A_\mu = a + n/2$ and

$$B_\mu = b + \frac{1}{2} \sum (x_i - \mu)^2 = n\hat{\sigma}^2 + n(\bar{x} - \mu)^2$$

where $\hat{\sigma}^2 = \frac{1}{n} \sum (x_i - \bar{x})^2$.

³do this on your own

Example

Goal: sample from $p(\mu, \lambda \mid x_{1:n})$

To implement Gibbs sampling in this example, each iteration consists of sampling:

$$\begin{aligned}\mu \mid \lambda, x_{1:n} &\sim \mathcal{N}(M_\lambda, L_\lambda^{-1}) \\ \lambda \mid \mu, x_{1:n} &\sim \text{Gamma}(A_\mu, B_\mu).\end{aligned}$$

This will give us samples

$$(\mu_0, \lambda_0), \dots, (\mu_S, \lambda_S)$$

Pareto example

Distributions of sizes and frequencies often tend to follow a “power law” distribution.

- ▶ wealth of individuals
- ▶ size of oil reserves
- ▶ size of cities
- ▶ word frequency
- ▶ returns on stocks

Power law distribution

The power law (also called the scaling law) states that a relative change in one quantity results in a proportional relative change in another.

Example: One simple example to think of is a square. If we double the length of one side, from 2 to 4 inches, then the area will quadruple (from 4 to 16 inches squared).

A power law distribution has the form

$$Y = kX^{\alpha}$$

, where:

X , Y are random variables, k is a constant and α is a fixed exponent.

Power law distribution

The Pareto distribution with shape $\alpha > 0$ and scale $c > 0$ has p.d.f.

$$\text{Pareto}(x|\alpha, c) = \frac{\alpha c^\alpha}{x^{\alpha+1}} \mathbb{1}(x > c) \propto \frac{1}{x^{\alpha+1}} \mathbb{1}(x > c).$$

- ▶ This is referred to as a power law distribution, because the p.d.f. is proportional to x raised to a power.
- ▶ c is a lower bound on the observed values.
- ▶ We will use Gibbs sampling to perform inference for α and c .
- ▶ Let X be the population of a city.

Pareto example

Rank	City	Population
1	Charlotte	731424
2	Raleigh	403892
3	Greensboro	269666
4	Durham	228330
5	Winston-Salem	229618
6	Fayetteville	200564
7	Cary	135234
8	Wilmington	106476
9	High Point	104371
10	Greenville	84554
11	Asheville	85712
12	Concord	79066
⋮	⋮	⋮
44	Havelock	20735
45	Carrboro	19582
46	Shelby	20323
47	Clemmons	18627
48	Lexington	18931
49	Elizabeth City	18683
50	Danville	17122

Parameter interpretations

- ▶ α tells us the scaling relationship between the size of cities and their probability of occurring.
 - ▶ Let $\alpha = 1$.
 - ▶ Density looks like $1/x^{\alpha+1} = 1/x^2$.
 - ▶ Cities with 10,000–20,000 inhabitants occur roughly $10^{\alpha+1} = 100$ times as frequently as cities with 100,000–110,000 inhabitants (or $10^{\alpha+1}/10 = 10$ times as frequently as cities with 100,000–200,000 inhabitants)
- ▶ c represents the cutoff point—any cities smaller than this were not included in the dataset.

Prior selection

For simplicity, let's use an **(improper) default prior**:

$$p(\alpha, c) \propto \mathbb{1}(\alpha, c > 0).$$

Recall:

- ▶ An *improper/default prior* is a non-negative function of the parameters which integrates to infinity.
- ▶ Often (but not always!) the resulting “posterior” will be proper.
- ▶ It is important that the “posterior” be proper, since otherwise the whole Bayesian framework breaks down.

Pareto example

Recall

$$p(x|\alpha, c) = \frac{\alpha c^\alpha}{x^{\alpha+1}} \mathbb{1}(x > c) \quad (2)$$

$$\mathbb{1}(\alpha, c > 0) \quad (3)$$

Let's derive the posterior:

$$\begin{aligned} p(\alpha, c|x_{1:n}) &\stackrel{\text{def}}{\propto}_{\alpha, c} p(x_{1:n}|\alpha, c)p(\alpha, c) \\ &\propto_{\alpha, c} \mathbb{1}(\alpha, c > 0) \prod_{i=1}^n \frac{\alpha c^\alpha}{x_i^{\alpha+1}} \mathbb{1}(x_i > c) \\ &= \frac{\alpha^n c^{n\alpha}}{(\prod x_i)^{\alpha+1}} \mathbb{1}(c < x_*) \mathbb{1}(\alpha, c > 0) \end{aligned} \quad (4)$$

where $x_* = \min\{x_1, \dots, x_n\}$.

Pareto example

As a joint distribution on (α, c) ,

- ▶ this does not seem to have a recognizable form,
- ▶ and it is not clear how we might sample from it directly.

Gibbs sampling

Let's try Gibbs sampling! To use Gibbs, we need to be able to sample $\alpha|c, x_{1:n}$ and $c|\alpha, x_{1:n}$.

By Equation 4, we find that

$$\begin{aligned} p(\alpha|c, x_{1:n}) &\propto_{\alpha} p(\alpha, c|x_{1:n}) \propto_{\alpha} \frac{\alpha^n c^{n\alpha}}{(\prod x_i)^{\alpha}} \mathbb{1}(\alpha > 0) \\ &= \alpha^n \exp(-\alpha(\sum \log x_i - n \log c)) \mathbb{1}(\alpha > 0) \\ &\propto_{\alpha} \text{Gamma}(\alpha | n + 1, \sum \log x_i - n \log c), \end{aligned}$$

and

$$p(c|\alpha, x_{1:n}) \propto_c p(\alpha, c|x_{1:n}) \propto_c c^{n\alpha} \mathbb{1}(0 < c < x_*),$$

which we will define to be $\text{Mono}(\alpha, x_*)$

Mono distribution

For $a > 0$ and $b > 0$, define the distribution $\text{Mono}(a, b)$ (for monomial) with p.d.f.

$$\text{Mono}(x|a, b) \propto x^{a-1} \mathbb{1}(0 < x < b).$$

Since $\int_0^b x^{a-1} dx = b^a/a$, we have

$$\text{Mono}(x|a, b) = \frac{a}{b^a} x^{a-1} \mathbb{1}(0 < x < b),$$

and for $0 < x < b$, the c.d.f. is

$$F(x|a, b) = \int_0^x \text{Mono}(y|a, b) dy = \frac{a}{b^a} \frac{x^a}{a} = \frac{x^a}{b^a}.$$

Pareto example

To use the inverse c.d.f. technique, we solve for the inverse of F on $0 < x < b$: Let $u = \frac{x^a}{b^a}$ and solve for x .

$$u = \frac{x^a}{b^a} \tag{5}$$

$$b^a u = x^a \tag{6}$$

$$bu^{1/a} = x \tag{7}$$

Can sample from $\text{Mono}(a, b)$ by drawing $U \sim \text{Uniform}(0, 1)$ and setting $X = bU^{1/a}$.⁴

⁴It turns out that this is an inverse of the Pareto distribution, in the sense that if $X \sim \text{Pareto}(\alpha, c)$ then $1/X \sim \text{Mono}(\alpha, 1/c)$.

Pareto example

So, in order to use the Gibbs sampling algorithm to sample from the posterior $p(\alpha, c | x_{1:n})$, we initialize α and c , and then alternately update them by sampling:

$$\begin{aligned}\alpha | c, x_{1:n} &\sim \text{Gamma}(n + 1, \sum \log x_i - n \log c) \\ c | \alpha, x_{1:n} &\sim \text{Mono}(n\alpha + 1, x_*).\end{aligned}$$

Traceplots

Traceplots. A traceplot simply shows the sequence of samples, for instance $\alpha_1, \dots, \alpha_N$, or c_1, \dots, c_N . Traceplots are a simple but very useful way to visualize how the sampler is behaving.

Traceplots

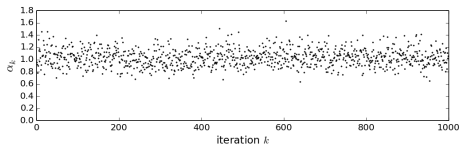


Figure 2: Traceplot of α

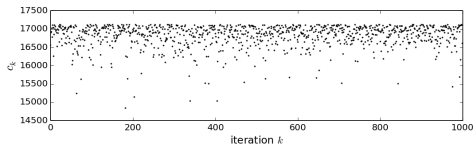


Figure 3: Traceplot of c .

Estimated density

Estimated density. We are primarily interested in the posterior on α , since it tells us the scaling relationship between the size of cities and their probability of occurring.

By making a histogram of the samples $\alpha_1, \dots, \alpha_N$, we can estimate the posterior density $p(\alpha|x_{1:n})$.

The two vertical lines indicate the lower ℓ and upper u boundaries of an (approximate) 90% credible interval $[\ell, u]$ —that is, an interval that contains 90% of the posterior probability:

$$\mathbb{P}(\alpha \in [\ell, u] | x_{1:n}) = 0.9.$$

Estimated density

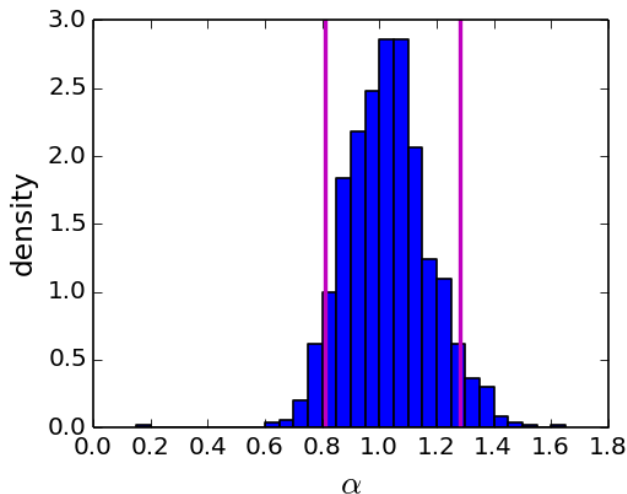


Figure 4: Estimated density of $\alpha|x_{1:n}$ with ≈ 90 percent credible intervals.

Running averages

Running averages. Panel (d) shows the running average $\frac{1}{k} \sum_{i=1}^k \alpha_i$ for $k = 1, \dots, N$.

In addition to traceplots, running averages such as this are a useful heuristic for visually assessing the convergence of the Markov chain.

The running average shown in this example still seems to be meandering about a bit, suggesting that the sampler needs to be run longer (but this would depend on the level of accuracy desired).

Running averages

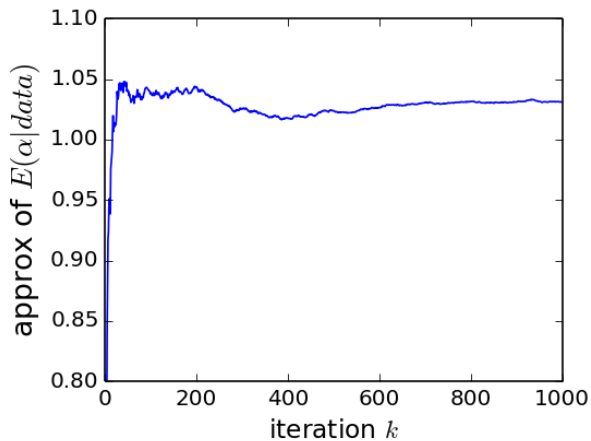


Figure 5: Running average plot

Survival functions

A survival function is defined to be

$$S(x) = \mathbb{P}(X > x) = 1 - \mathbb{P}(X \leq x).$$

Power law distributions are often displayed by plotting their survival function $S(x)$, on a log-log plot.

Why? $S(x) = (c/x)^\alpha$ for the $\text{Pareto}(\alpha, c)$ distribution and on a log-log plot this appears as a line with slope $-\alpha$.

The posterior survival function (or more precisely, the posterior predictive survival function), is $S(x|x_{1:n}) = \mathbb{P}(X_{n+1} > x \mid x_{1:n})$.

Survival functions

Figure 6(e) shows an empirical estimate of the survival function (based on the empirical c.d.f., $\hat{F}(x) = \frac{1}{n} \sum_{i=1}^n \mathbb{1}(x \geq x_i)$) along with the posterior survival function, approximated by

$$S(x|x_{1:n}) = \mathbb{P}(X_{n+1} > x \mid x_{1:n}) \quad (8)$$

$$= \int \mathbb{P}(X_{n+1} > x \mid \alpha, c) p(\alpha, c | x_{1:n}) d\alpha dc \quad (9)$$

$$\approx \frac{1}{N} \sum_{i=1}^N \mathbb{P}(X_{n+1} > x \mid \alpha_i, c_i) = \frac{1}{N} \sum_{i=1}^N (c_i/x)^{\alpha_i}. \quad (10)$$

This is computed for each x in a grid of values.

Survival functions

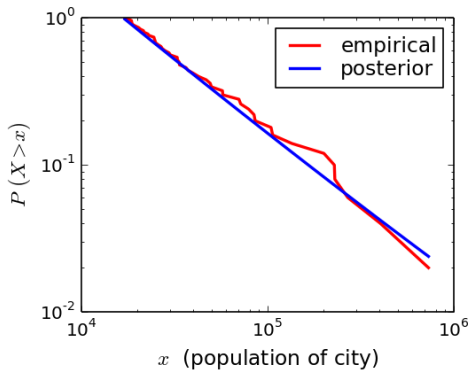


Figure 6: Empirical vs posterior survival function

Detailed Takeways

- ▶ inverse CDF method
- ▶ Two-stage Gibbs sampler
- ▶ Markov Chain
- ▶ properties of Markov chains
- ▶ Exponential Example
- ▶ Truncated Exponential
- ▶ Normal-Normal-Gamma
- ▶ Pareto Case Study
- ▶ Trace plots
- ▶ Estimated Densities
- ▶ Running Average Plots
- ▶ Survival Functions