Module 7: Introduction to Gibbs Sampling

Rebecca C. Steorts

Agenda

- Gibbs sampling
- Exponential example
- Normal example
- Pareto example

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 $X \mid Y = y_0$.
   Current state: (x_1, y_0)
   Sample $y_1 \sim p(y|x_1)$, that is, from the conditional distribution $Y \mid X = x_1$.
   Current state: (x_1, y_1)
2. Sample $x_2 \sim p(x|y_1)$, that is, from the conditional distribution $X \mid Y = y_1$.
   Current state: (x_2, y_1)
   Sample $y_2 \sim p(y|x_2)$, that is, from the conditional distribution $Y \mid X = x_2$.
   Current state: (x_2, y_2)
   $\vdots$

Repeat iterations 1 and 2, M times.

Gibbs sampler

This procedure defines a sequence of pairs of random variables

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

Markov chain and dependence

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

satisfies the property of being a Markov chain.

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

$(X_0, Y_0), (X_1, Y_1), (X_2, Y_2), (X_3, Y_3), \ldots$ 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 $(X_1, Y_1), \ldots, (X_B, Y_B)$. 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) $x = (x_1, \ldots, x_n)$.[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 $p(a, b|x)$.

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

Conditional distributions

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

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

Conditional distributions

This conditional distribution satisfies

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

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,] 0.250000 0.2500000
## [2,] 1.651202 0.2970126
## [3,] 1.412094 0.3807388
## [4,] 1.588245 0.2890392
## [5,] 1.652233 0.3254774
## [6,] 1.641554 0.3946844
```

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

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

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

- $p(x|y)$ 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.

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

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 $u \in (0, 1)$.

Hint: To verify the last step: apply the rejection principle (along with the inverse cdf technique). Verify the last step on your own.

Toy example

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

0. Initialize $x_0, y_0 \in S$.
1. Sample $x_1 \sim \mathrm{TExp}(y_0, S)$, then sample $y_1 \sim \mathrm{TExp}(x_1, S)$.
2. Sample $x_2 \sim \mathrm{TExp}(y_1, S)$, then sample $y_2 \sim \mathrm{TExp}(x_2, S)$.

   $\vdots$

N. Sample $x_N \sim \mathrm{TExp}(y_{N-1}, S)$, sample $y_N \sim \mathrm{TExp}(x_N, S)$.

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

Toy example

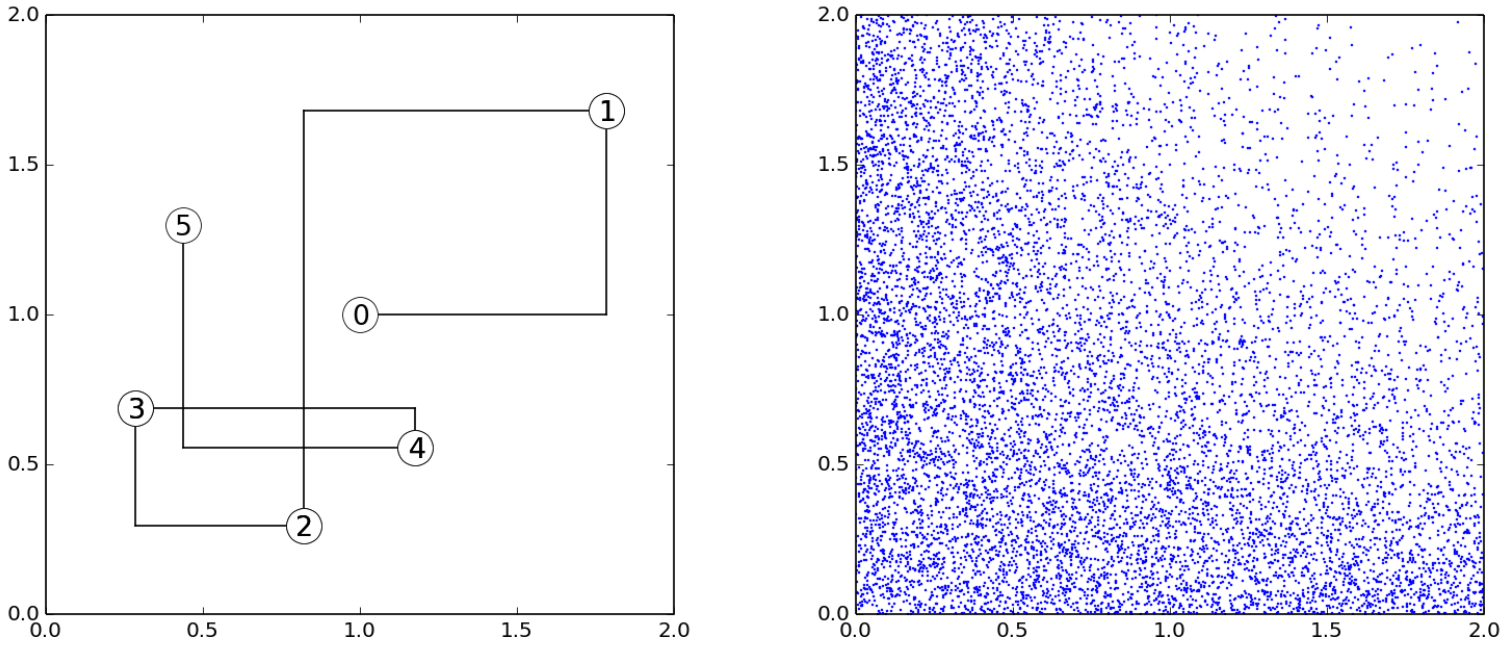

Figure 1: (Left) Schematic representation of the first 5 Gibbs sampling iterations/sweeps/scans. (Right) Scatterplot of samples from 10^4 Gibbs sampling iterations.

Example: Normal with semi-conjugate prior

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

$$\boldsymbol{\mu} \sim \mathcal{N}(\mu_0, \lambda_0^{-1})$$
$$\boldsymbol{\lambda} \sim \text{Gamma}(a, b)$$

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 $x_{1:n}$.

Example

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

$$\boldsymbol{\mu}|\lambda, x_{1:n} \sim \mathcal{N}(M_\lambda, L_\lambda^{-1})$$

where

$$L_\lambda = \lambda_0 + n\lambda \text{ and } M_\lambda = \frac{\lambda_0\mu_0 + \lambda\sum_{i=1}^n x_i}{\lambda_0 + n\lambda}.$$

For any fixed value of μ, it is straightforward to derive[3] that

$$\boldsymbol{\lambda}|\mu, x_{1:n} \sim \text{Gamma}(A_\mu, B_\mu) \tag{1}$$

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

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

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

[3] do this on your own

Example

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

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

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 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.

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

Parameter intepretations

- 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.
- 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

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

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

Let's derive the posterior:

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

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

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

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

and

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

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

Mono distribution

For $a > 0$ and $b > 0$, define the distribution 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.

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

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

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

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

[4] It turns out that this is an inverse of the Pareto distribution, in the sense that if $X \sim$ Pareto(α, c) then $1/X \sim$ 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:

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

Traceplots

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

Traceplots

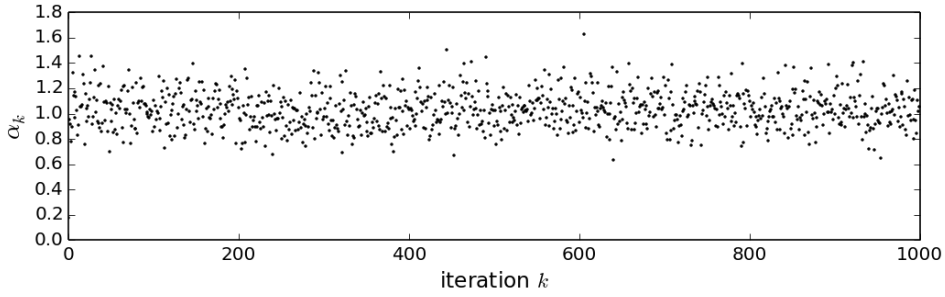

Figure 2: Traceplot of α

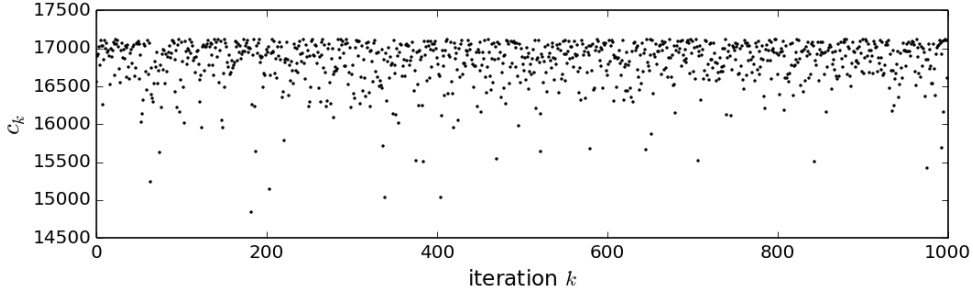

Figure 3: Traceplot of c.

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 $\alpha_1, \ldots, \alpha_N$, 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:

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

Estimated density

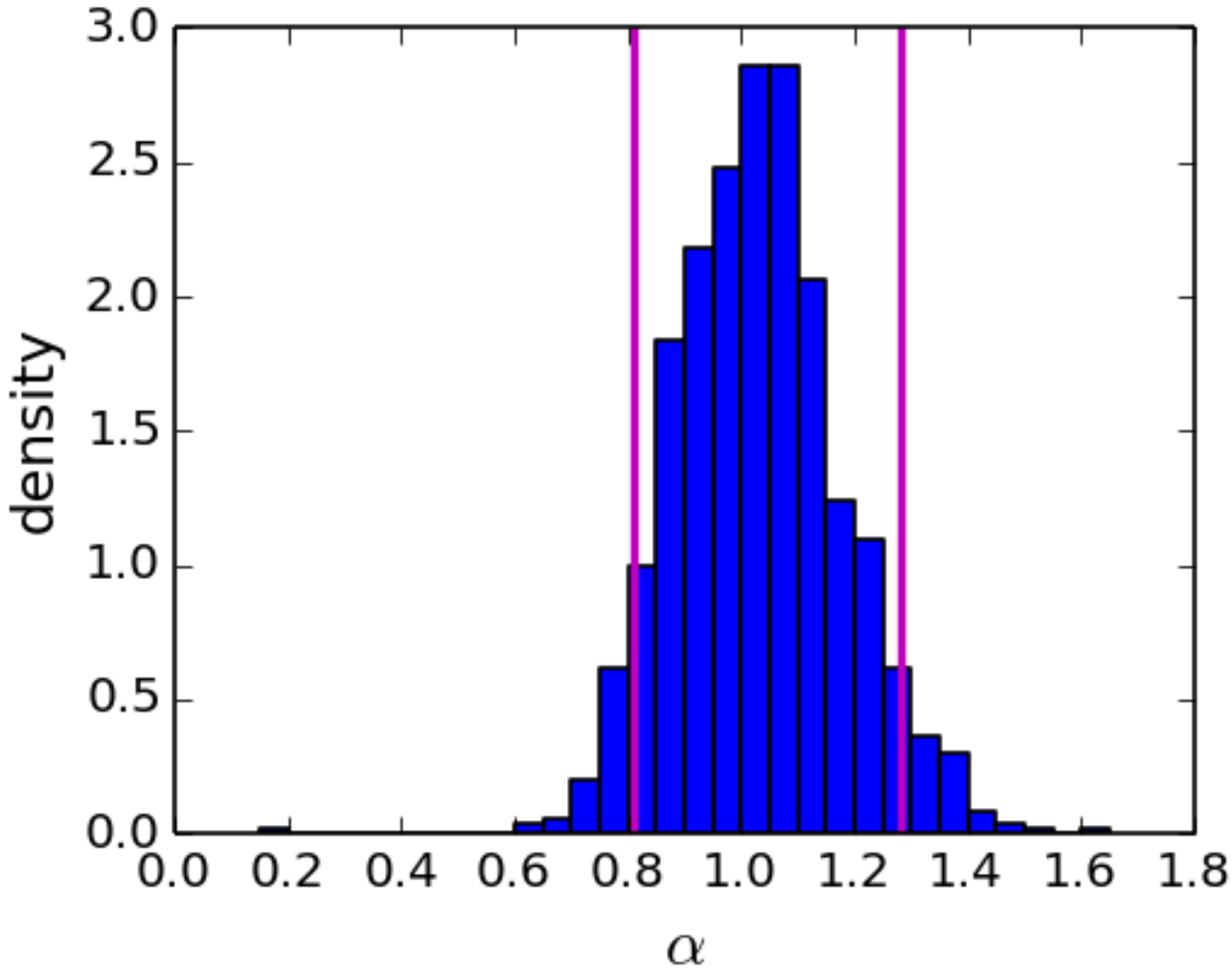

Figure 4: Estimated density of $\alpha|x_{1:n}$ with $\approx$ 90 percent credible intervals.

Running averages

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

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

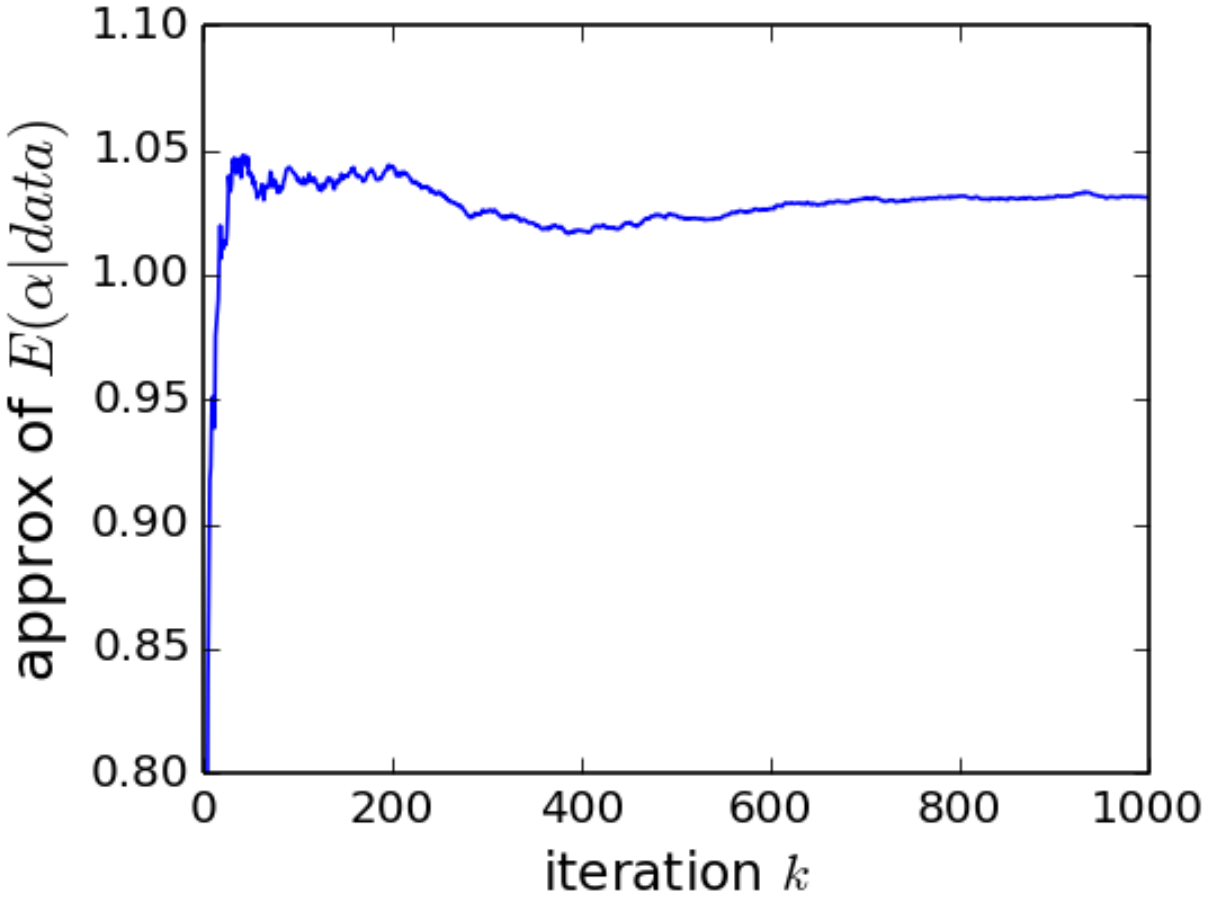

Figure 5: Running average plot

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 Pareto(α, 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

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

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

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

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

Survival functions

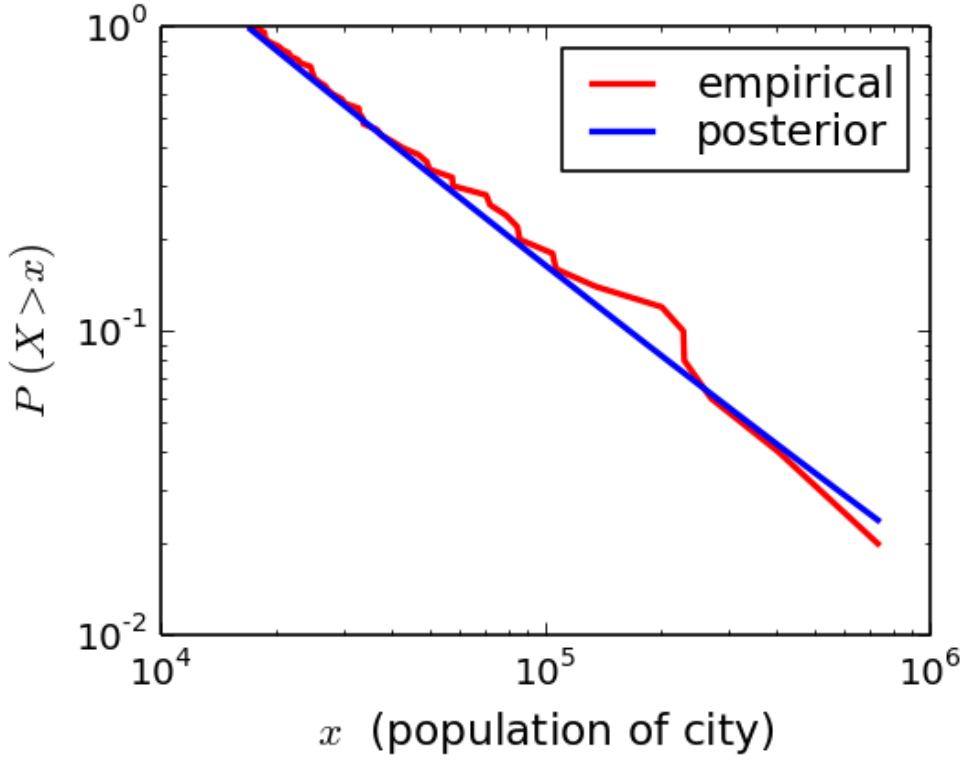

Figure 6: Empirical vs posterior survival function

How could we get a better empirical approximation?

Multi-stage Gibbs sampler

Assume three random variables, with joint pmf or pdf: $p(x, y, z)$..

Set x, y, and z to some values (x_o, y_o, z_o).

Sample $x|y, z$, then $y|x, z$, then $z|x, y$, then $x|y, z$, and so on. More precisely,

0. Set (x_0, y_0, z_0) to some starting value.
1. Sample $x_1 \sim p(x|y_0, z_0)$.
   Sample $y_1 \sim p(y|x_1, z_0)$.
   Sample $z_1 \sim p(z|x_1, y_1)$.
2. Sample $x_2 \sim p(x|y_1, z_1)$.
   Sample $y_2 \sim p(y|x_2, z_1)$.
   Sample $z_2 \sim p(z|x_2, y_2)$.
   $\vdots$

Multi-stage Gibbs sampler

Assume d random variables, with joint pmf or pdf $p(v^1, \ldots, v^d)$.

At each iteration $(1, \ldots, M)$ of the algorithm, we sample from

$$
\begin{aligned}
v^1 &\mid v^2, v^3, \ldots, v^d \\
v^2 &\mid v^1, v^3, \ldots, v^d \\
&\vdots \\
v^d &\mid v^1, v^2, \ldots, v^{d-1}
\end{aligned}
$$

always using the most recent values of all the other variables.

The conditional distribution of a variable given all of the others is referred to as the *full conditional* in this context, and for brevity denoted $v^i | \cdots$.

Example: Censored data

In many real-world data sets, some of the data is either missing altogether or is partially obscured.

One way in which data can be partially obscured is by *censoring*, which means that we know a data point lies in some particular interval, but we don't get to observe it exactly.

Medical data censoring

6 patients participate in a cancer trial, however, patients 1, 2 and 4 leave the trial early. Then we know when they leave the study, but we don't know information about them as the trial continues.

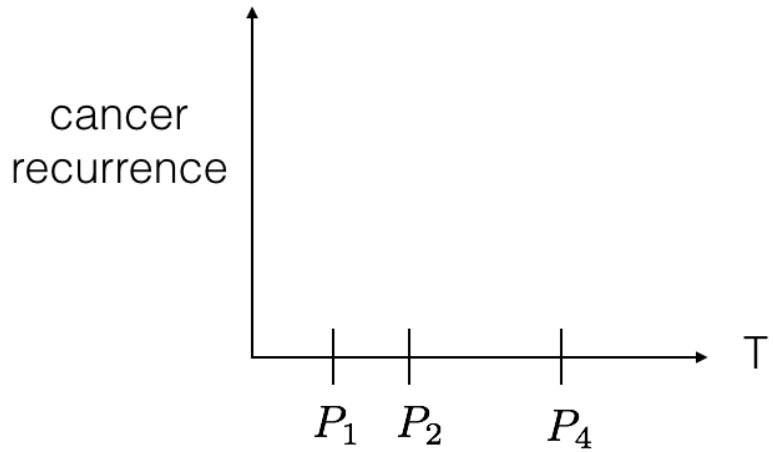

Figure 7: Example of censoring for medical data.

This is a certain type of missing data.

Heart Disease (Censoring) Example

- Researchers are studying the length of life (lifetime) following a particular medical intervention, such as a new surgical treatment for heart disease.
- The study consists of 12 patients.
- The number of years before death for each is

$$3.4, 2.9, 1.2+, 1.4, 3.2, 1.8, 4.6, 1.7+, 2.0+, 1.4+, 2.8, 0.6+$$

where $x+$ indicates that the patient was alive after x years, but the researchers lost contact with the patient at that point.

Model

$$X_i = \begin{cases} Z_i & \text{if } Z_i \leq c_i \\ * & \text{if } Z_i > c_i \end{cases} \tag{11}$$

$$Z_1, \ldots, Z_n | \theta \overset{iid}{\sim} \text{Gamma}(r, \theta) \tag{12}$$

$$\theta \sim \text{Gamma}(a, b) \tag{13}$$

where a, b, and r are known, and $*$ is a special value to indicate that censoring has occurred.

- X_i is the observation
  - if the lifetime is less than c_i then we get to observe it ($X_i = Z_i$),
  - otherwise all we know is the lifetime is greater than c_i ($X_i = *$).
- θ is the parameter of interest—the rate parameter for the lifetime distribution.
- Z_i is the lifetime for patient i, however, this is not directly observed.
- c_i is the censoring time for patient i, which is fixed, but known only if censoring occurs.

Gibbs saves again!

Straightforward approaches that are in closed form don't seem to work (think about these on your own). Instead we turn to GS.

To sample from $p(\theta, z_{1:n}|x_{1:n})$, we cycle through each of the full conditional distributions,

$$\begin{aligned}
\theta &\mid z_{1:n}, x_{1:n} \\
z_1 &\mid \theta, z_{2:n}, x_{1:n} \\
z_2 &\mid \theta, z_1, z_{3:n}, x_{1:n} \\
&\vdots \\
z_n &\mid \theta, z_{1:n-1}, x_{1:n}
\end{aligned}$$

sampling from each in turn, always conditioning on the most recent values of the other variables.

Gibbs

Recall

$$X_i = \begin{cases} Z_i & \text{if } Z_i \leq c_i \\ * & \text{if } Z_i > c_i \end{cases} \tag{14}$$

$$Z_1, \ldots, Z_n | \theta \overset{iid}{\sim} \text{Gamma}(r, \theta) \tag{15}$$

$$\theta \sim \text{Gamma}(a, b) \tag{16}$$

The full conditionals are easy to calculate. Let's start with $\theta | \cdots$

- Since $\theta \perp x_{1:n} \mid z_{1:n}$ (i.e., θ is conditionally independent of $x_{1:n}$ given $z_{1:n}$),

$$p(\theta | \cdots) = p(\theta | z_{1:n}, x_{1:n}) = p(\theta | z_{1:n}) \tag{17}$$

$$= \text{Gamma}\left(\theta \,\middle|\, a + nr,\ b + \textstyle\sum_{i=1}^{n} z_i\right) \tag{18}$$

  using the fact that the prior on θ is conjugate.

Full conditionals

Now let's move to z? What happens here? This is the start of **Homework 6.**

1. Find the full conditional for $(z_i \mid \cdots)$.
2. Code up your own multi-stage GS in R. Be sure to use efficient functions.
3. Use the censored data

$$3.4, 2.9, 1.2+, 1.4, 3.2, 1.8, 4.6, 1.7+, 2.0+, 1.4+, 2.8, 0.6+$$

. Specifically, give (a) give traceplots of all unknown paramaters from the G.S. (b) a running average plot, (c) the estimated density of $\theta \mid \cdots$ and $z_9 \mid \cdots$. Be sure to give brief explanations of your results.