Gibbs Samplers

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Introduction

Now that we've familiarized ourselves with MCMC and the Metropolis-Hastings algorithms, we begin to analyze a now-common MCMC algorithm called Gibbs sampler. The Gibbs sampler is in fact a special case of the Metropolis-Hastings algorithm for high dimensional target distributions.

Recommended reading: Explaining the Gibbs Sampler

Two-stage Gibbs sampler algorithm

The Gibbs sampler creates a Markov chain from a joint distribution in the following way. If two random variables X and Y have joint density $f(x, y)$, with corresponding conditional densities $f_{Y|X}$ and $f_{X|Y}$, the two stage Gibbs sampler generates a Markov chain (X_t, y_i) by generating y_i from conditional density $f_{Y|X}$ and then generating X_t from conditional density $f_{X|Y}$.

The **two-stage Gibbs sampler algorithm** as described Robert & Casella goes as follows

```
Take $X_0 = x_0$

For $t = 1, 2, \ldots$, generate

1. $y_i \sim f_{Y|X}(\cdot|x_{t-1})$

2. $X_t \sim f_{X|Y}(\cdot|y_t)$
```

Bivariate Normal Example

We illustrate the implementation of the Gibbs sampler with a simple example. Consider a bivariate Normal distribution where

$$X, Y \sim N_2\left(\begin{pmatrix}\mu_X \\ \mu_Y\end{pmatrix}, \ \begin{pmatrix}\sigma_X^2 & \sigma_{XY}^2 \\ \sigma_{YX}^2 & \sigma_Y^2\end{pmatrix}\right)$$

Bivariate Normal Example

The marginal distributions of X and Y are $N(\mu_X, \sigma_X)$ and $N(\mu_X, \sigma_X)$. The conditional distributions of Y and X are

$$Y|X = x \sim N\left(\mu_Y + \frac{\rho\sigma_Y}{\sigma_X}(x - \mu_X), (1-\rho^2)\sigma_Y^2\right)$$

and

$$X|Y = y \sim N\left(\mu_X + \frac{\rho\sigma_X}{\sigma_Y}(y - \mu_Y), (1-\rho^2)\sigma_X^2\right)$$

ρ is the correlation between X and Y, and $(1-\rho^2)\sigma_X^2$ is the variance.

Multivariate Normal Distribution

Bivariate Normal Example

```
library(MASS, quietly = TRUE) ## for kernel density estimation
library(RColorBrewer, quietly = TRUE) ## some pretty colors
k <- 11
my.cols <- rev(brewer.pal(k, "RdYlBu"))

N = 100000
rho = 0.9
mu_x = 1
mu_y = 2
sd_x = 1.2
sd_y = 0.75

s1 = sqrt(1 - rho^2) * sd_x
s2 = sqrt(1 - rho^2) * sd_y

MVN = matrix(data = NA, nrow = N, ncol = 2,
           dimnames = list(NULL, c("X", "Y")))
```

Bivariate Normal Example

```
MVN[1, ] = c(mu_x, mu_y)
Y = MVN[1, 2] ## get Y vals
for(i in 1:(N-1)){
  mx = mu_x + rho * (Y - mu_y) * sd_x/sd_y
  X = rnorm(n = 1, mx, s1)
  MVN[i+1, 1] = X
  my = mu_y + rho * (X - mu_x) * sd_y/sd_x
  Y = rnorm(n = 1, mean = my, sd = s2)
  MVN[i+1, 2] = Y
}


## means
colMeans(MVN)
```

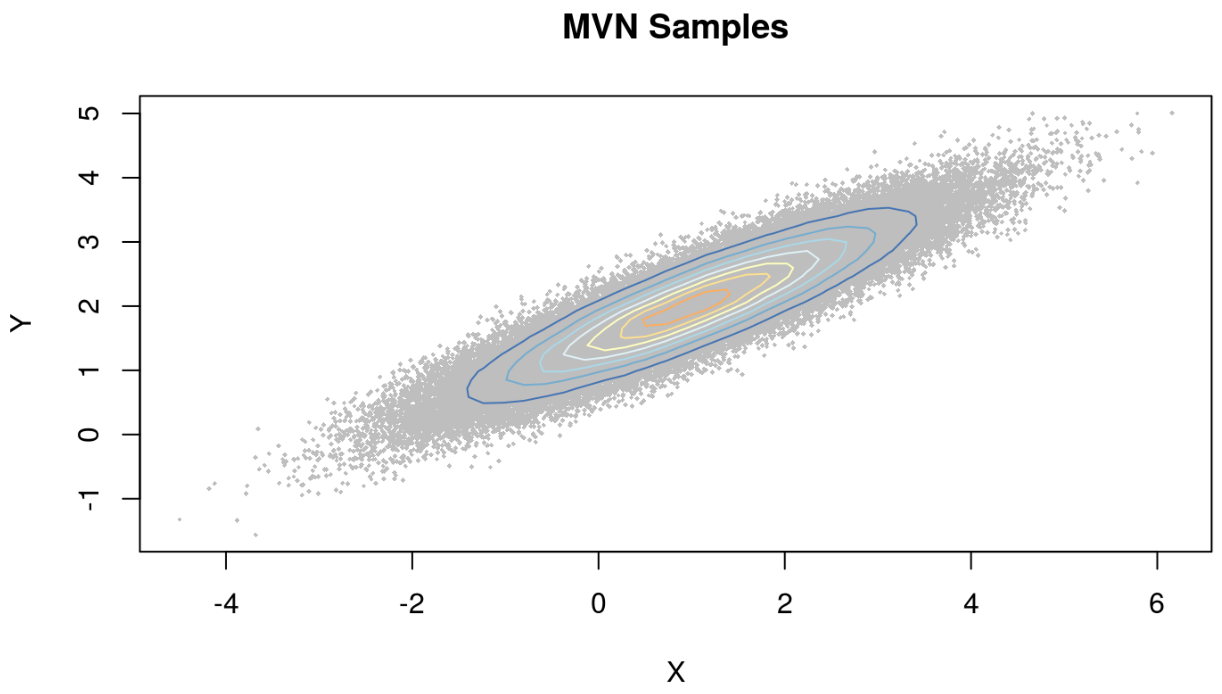
```
##        X        Y
## 1.000312 1.999968
```

```
## correlation
cor(MVN)
```

```
##           X         Y
## X 1.0000000 0.9011088
## Y 0.9011088 1.0000000
```

Bivariate Normal Example

```
z = kde2d(x = MVN[,1], y = MVN[,2], n = 50) ## kernel density estimation
plot(MVN, xlab="X", ylab="Y", pch = 18, col = 8, cex=.4, main = "MVN Samples")
contour(z, drawlabels=FALSE, nlevels=k, col=my.cols, add=TRUE) ## add contours to plot
```



Beta-Binomial revisited

In the introduction to these notes, we saw a Bayesian example of the Beta-Binomial distribution. From Casella's paper , we revisit this example.

$$X|\theta \sim Bin(n, \theta), \text{ and } \theta \sim Beta(a, b)$$

have joint density

$$f(x, \theta) = \binom{n}{x} \frac{\Gamma(a+b)}{\Gamma(a)\Gamma(b)} \theta^{x+a-1} (1-\theta)^{n-x+b-1}$$

is the a $Beta(x+a, n-x+b)$ distribution.

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Beta-Binomial revisited

Suppose we are interested in calculating some characteristics of the marginal distributions of $X|\theta$ and $\theta|a, b, x, n$.

$$f(x|\theta) \text{ is } Bin(n, \theta)$$
$$f(\theta|x) \text{ is } Beta(x+a, n-x+b)$$

Therefore, we follow an iterative algorithm of

$$X_i \sim f(x|\theta)$$
$$\theta_{i+1} \sim f(\theta|X_i = x_i)$$

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Beta-Binomial revisited

```r
n = 16
a = 2
b = 4
X = numeric(N)
thetas = numeric(N)

X[1] = runif(1) ## initial values
thetas[1] = runif(1) ## theta values

for(i in 1:N){
  X[i+1] = rbinom(n = 1, size = n, prob = thetas[i])
  thetas[i+1] = rbeta(1, a + X[i+1], n - X[i+1]+b)
}

quantile(X)
```

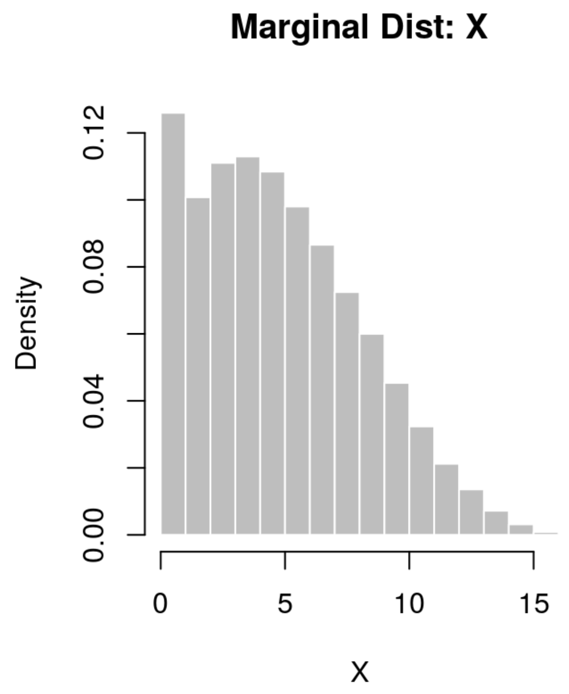
```
##   0%  25%  50%  75% 100% 
##    0    3    5    8   16
```

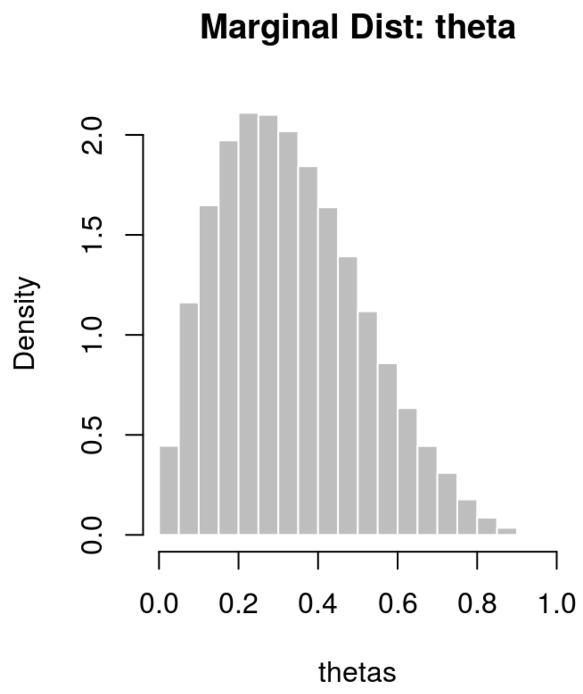
```r
quantile(thetas)
```

```
##           0%          25%          50%          75%         100% 
## 0.0005819406 0.1944846157 0.3136805137 0.4520986182 0.9659229861
```

Beta-Binomial revisited

```
par(mfrow = c(1,2))
hist(X, main = "Marginal Dist: X", probability = TRUE, border = "white", col = "gray")
hist(thetas, main = paste("Marginal Dist:", expression(theta)), probability = TRUE, border = "white", col = "gray")
```





The multistage Gibbs sampler

There is a natural extension from the two-stage Gibs sampler to the general multistage Gibbs sampler. Suppose that, for some $p > 1$, the random variable $\mathbf{X} \in X$ can be written as $\mathbf{X} = (X_1, \ldots, X_p)^T$ where the X_i's are either unidimensional or multidimensional components. Suppose that we can simulate from the corresponding conditional densities, $f_1, f_2, \ldots, f_p$ that is, we can simulate

$$X_i|x_1, \ldots, x_{i-1}, x_{i+1}, \ldots, x_p \sim f(x_i|x_1, \ldots, x_{i-1}, x_{i+1}, \ldots, x_p)$$

for i in 1, 2, …, p. THe associated Gibbs sampler is given as

The multistage Gibbs sampler

At iteration $t = 1, 2, \ldots$, given $\mathbf{x^{(t)}} = (x^{(1)}, \ldots, x^{(p)})$, generate

1. $X_1^{(t+1)} \sim f_1(x_1 | x_2^{(t)}, \ldots, x_p^{(t)})$

2. $X_2^{(t+1)} \sim f_2(x_2 | x_1^{(t+1)}, x_3^{(t)} \ldots, x_p^{(t)})$
…

p. $X_p^{(t+1)} \sim f_p(x_p | x_1^{(t+1)}, \ldots, x_{p-1}^{(t+1)})$.

The densities $f_1, \ldots, f_p$ are called the , and a particular feature of teh Gibbs sampler is that these are the only densities used for simulation. Thus, even in a high-dimensional problem, all of the simulations be univariate, which can be a huge advantage!

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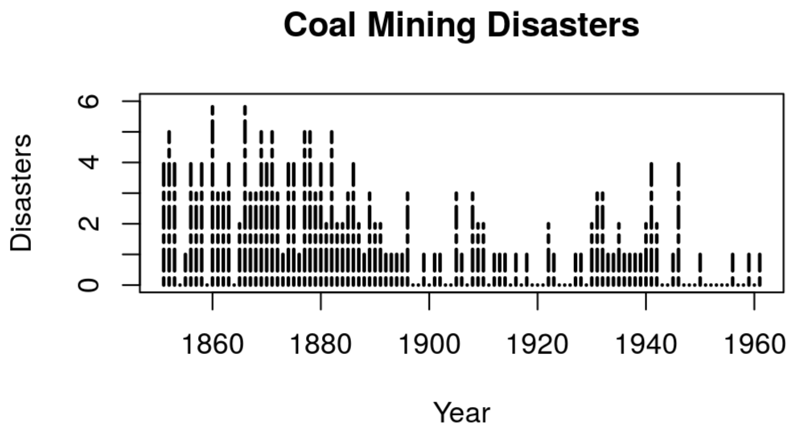
Bayesian Change-Point Analysis

Let's try to model a more interesting example, a time series of recorded coal mining disasters in the UK from 1851 to 1962, for $n = 111$ years of data. This analysis will follow the analysis layed out by Carlin et al in Hierarchical Bayesian Analysis of Changepoint Problems. Occurrences of disasters in the time series is thought to be derived from a Poisson process with a drop rate parameter in the later part of the time series. We are interested in locating the change point, k, in the series.

Change Point Detection

Bayesian Change-Point Analysis

```
data_vector = c(4, 5, 4, 0, 1, 4, 3, 4, 0, 6, 3, 3, 4, 0, 2, 6,
                3, 3, 5, 4, 5, 3, 1, 4, 4, 1, 5, 5, 3, 4, 2, 5,
                2, 2, 3, 4, 2, 1, 3, 2, 2, 1, 1, 1, 1, 3, 0, 0,
                1, 0, 1, 1, 0, 0, 3, 1, 0, 3, 2, 2, 0, 1, 1, 1,
                0, 1, 0, 1, 0, 0, 0, 2, 1, 0, 0, 0, 1, 1, 0, 2,
                3, 3, 1, 1, 2, 1, 1, 1, 1, 2, 4, 2, 0, 0, 1, 4,
                0, 0, 0, 1, 0, 0, 0, 0, 0, 1, 0, 0, 1, 0, 1)
n = length(data_vector)
disasters = ts(data_vector, freq=1, start = 1851)
plot(disasters, type = "h", lty = 6, lwd = 2, main = "Coal Mining Disasters", xlab = "Year", ylab = "Disasters")
```



Bayesian Change-Point Analysis

We are going to use Poisson random variables for this type of count data. Denoting year i's accident count by y_i,

$$y_i \sim \text{Poisson}(\Lambda)$$

The modeling problem revolves around estimating the values of the λ parameters. Looking at the time series above, it appears that the rate declines later in the time series. A changepoint model identifies a point (year) during the observation period (k) after which the parameter λ drops to a lower value. So we are estimating two λ parameters: one for the early period and another for the late period.

$$\Lambda = \begin{cases} \theta \text{ if } i < k \\ \lambda \text{ if } i \geq k \end{cases}$$

Bayesian Change-Point Analysis

We need to assign prior probabilities to both θ and λ parameters. The gamma distribution not only provides a continuous density function for positive numbers, but it is also conjugate with the Poisson sampling distribution.

We will specify suitably vague hyperparameters, letting $\alpha = 1$ and allowing βs to vary.

$$\theta \sim \text{Gamma}(1, b_1)$$
$$\lambda \sim \text{Gamma}(1, b_2)$$

Bayesian Change-Point Analysis

Since we do not have any intuition about the location of the changepoint (prior to viewing the data), we will assign a discrete uniform prior over all years 1851-1962.

$$k \sim \text{Unif}(1851{,}1962)$$

$$\Rightarrow p(K = k) = \frac{1}{111}$$

Implementing Gibbs sampling

We are interested in estimating the joint posterior of θ, λ and k given the array of annnual disaster counts $\mathbf{y}$. This gives:

$$p(\theta, \lambda, k|\mathbf{y}) \propto p(\mathbf{y}|\theta, \lambda, k)p(\theta, \lambda, k)$$

To employ Gibbs sampling, we need to factor the joint posterior into the product of conditional expressions:

$$p(\theta, \lambda, k|\mathbf{y}) \propto p(y_{i<k}|\theta, k)p(y_{i\geq k}|\lambda, k)p(\theta)p(\lambda)p(k)$$

which we have specified as:

$$\begin{aligned} p(\theta, \lambda, k|\mathbf{y}) &\propto \left[\prod_{t=1851}^{k} \text{Poisson}(y_i|\theta) \times \prod_{t=k+1}^{1962} \text{Poisson}(y_i|\lambda)\right] \times \text{Gamma}(\theta|\alpha, \beta) \times \text{Gamma}(\lambda|\alpha, \beta)\frac{1}{111} \\ &\propto \left[\prod_{t=1851}^{k} e^{-\theta}\theta^{y_i} \prod_{t=k+1}^{1962} e^{-\lambda}\lambda^{y_i}\right] \theta^{\alpha-1}e^{-\beta\theta}\lambda^{\alpha-1}e^{-\beta\lambda} \\ &\propto \theta^{\sum_{t=1851}^{k} y_i+\alpha-1}e^{-(\beta+k)\theta}\lambda^{\sum_{t=k+1}^{1962} y_i+\alpha-1}e^{-\beta\lambda} \end{aligned}$$

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Implementing Gibbs sampling

So, the full conditionals are known, and critically for Gibbs, can easily be sampled from.

$$\theta \sim \text{Gamma}\left(\sum_{t=1851}^{k} y_i + \alpha, k + \beta\right)$$

$$\lambda \sim \text{Gamma}\left(\sum_{t=k+1}^{1962} y_i + \alpha, 1962 - k + \beta\right)$$

$$p(k|\mathbf{y}, \theta, \lambda, b_1, b_2) = \frac{L(\mathbf{y}|\theta, \lambda, b_1, b_2)}{\sum_{j=1}^{n} L(\mathbf{y}|\theta, \lambda, b_1, b_2)}$$

where the likelihood is defined as

$$L(\mathbf{y}|\theta, \lambda, b_1, b_2) = e^{(\lambda-\theta)}\left(\frac{\theta}{\lambda}\right)^{\sum_1^k y_i}$$

Implementing Gibbs sampling

```
set.seed(123)

y = data_vector
# Gibbs sampler for the coal mining change point
# initialization
n <- length(y) #length of the data
m <- 10^4 #length of the chain

## vectors to hold data
theta <- numeric(m)
lambda <- numeric(m)
k <- numeric(m)
L <- numeric(n)

## initial values
k[1] <- sample(1:n, 1) ## change-points
theta[1] <- 1
lambda[1] <- 1
a = 0.5
b1 <- 1
b2 <- 1
```

Implementing Gibbs sampling

The algorithm explained by Carlin et al is simple. For $t \in \{1, 2, \dots, m\}$

1. Sample $\theta_t \sim Gamma(a_1 + \sum_1^k y_i, k_{t-1} + b_{1,t-1})$
2. Sample $\lambda_t \sim Gamma(a_2 + \sum_{k+1}^n y_i, n - k_{t-1} + b_{2,t-1})$
3. Sample $b_1 \sim Gamma(a_1 + c_1, (\theta_t + d_1))$
4. Sample $b_2 \sim Gamma(a_2 + c_2, (\lambda_t + d_2))$
5. For $j \in 1, \dots, n$ calculate $L(\mathbf{y}|\theta, \lambda, b_1, b_2)$, from there you'll obtain $p(k|\mathbf{y}, \theta, \lambda, b_1, b_2)$
6. Sample $k_t \sim p(k|\mathbf{y}, \theta, \lambda, b_1, b_2)$

Implementing Gibbs sampling

```
# run the Gibbs sampler
for (t in 2:m){
    kt <- k[t-1]
    #generate theta
    r <- a + sum(y[1:kt])
    theta[t] <- rgamma(1, shape = r, rate = kt + b1)
    #generate lambda
    if (kt + 1 > n){
      r <- a + sum(y)
      }else{
        r <- a + sum(y[(kt+1):n])
      }
    lambda[t] <- rgamma(1, shape = r, rate = n - kt + b2)
    #generate b1 and b2
    b1 <- rgamma(1, shape = a, rate = theta[t]+1)
    b2 <- rgamma(1, shape = a, rate = lambda[t]+1)

    for (j in 1:n) {
        L[j] <- exp((lambda[t] - theta[t]) * j) *
                (theta[t] / lambda[t])^sum(y[1:j])
    }
    L <- L / sum(L)
    #generate k from discrete distribution L on 1:n
    k[t] <- sample(1:n, prob=L, size=1)
}
```

Implementing Gibbs sampling

Set a burn-in of 1000 samples. We will use burn in to toss out "poor" samples from out Markov chain. Arguments for and against burn-in vary. Statisticians, Andrew Gelman (Burn-in Man) and Charlie Geyer (Burn-In) provide some commentary on burn-in.

```
## set burn in
burn_in <- 1000
## will toss out first 1000 samples

K <- k[burn_in:m]

## mean
print(mean(K))
```

```
## [1] 39.82791
```

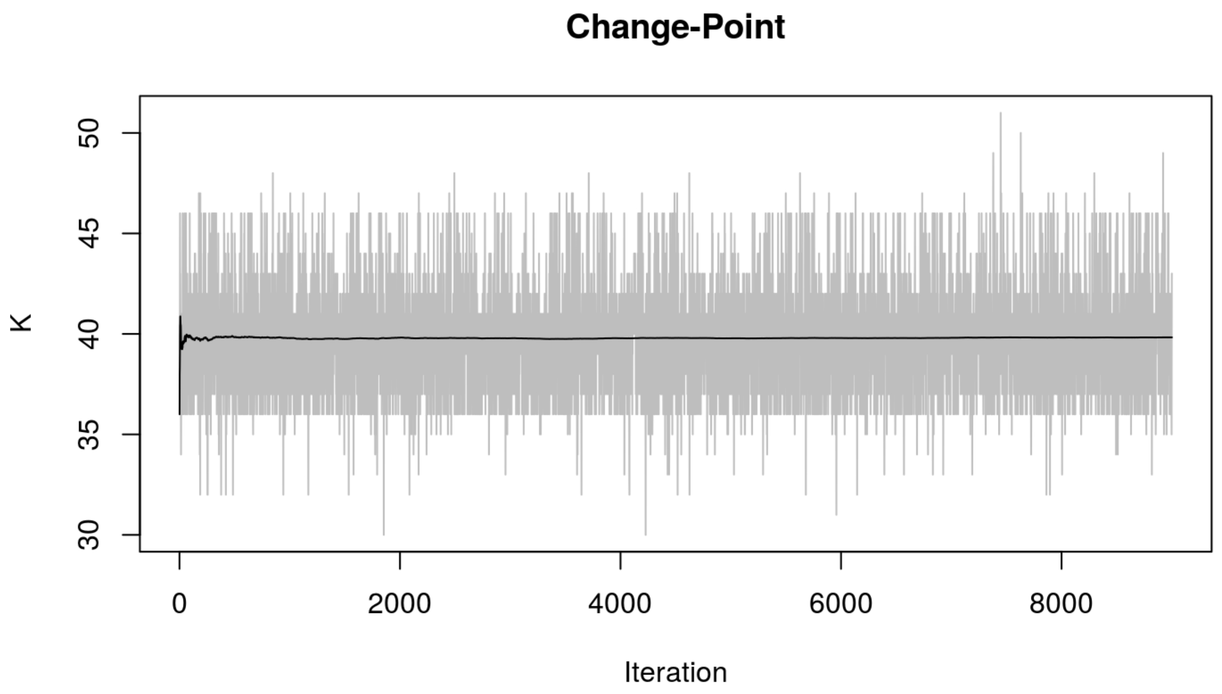
```
#[1] 39.935

## mode
print(which.max(table(K)))
```

```
## 41
## 12
```

Implementing Gibbs sampling

```r
plot(K, type="l", col="gray", main = "Change-Point",
     xlab="Iteration", ylab = "K")
lines(1:length(K), cumsum(K) / (1:length(K)))
```



Implementing Gibbs sampling

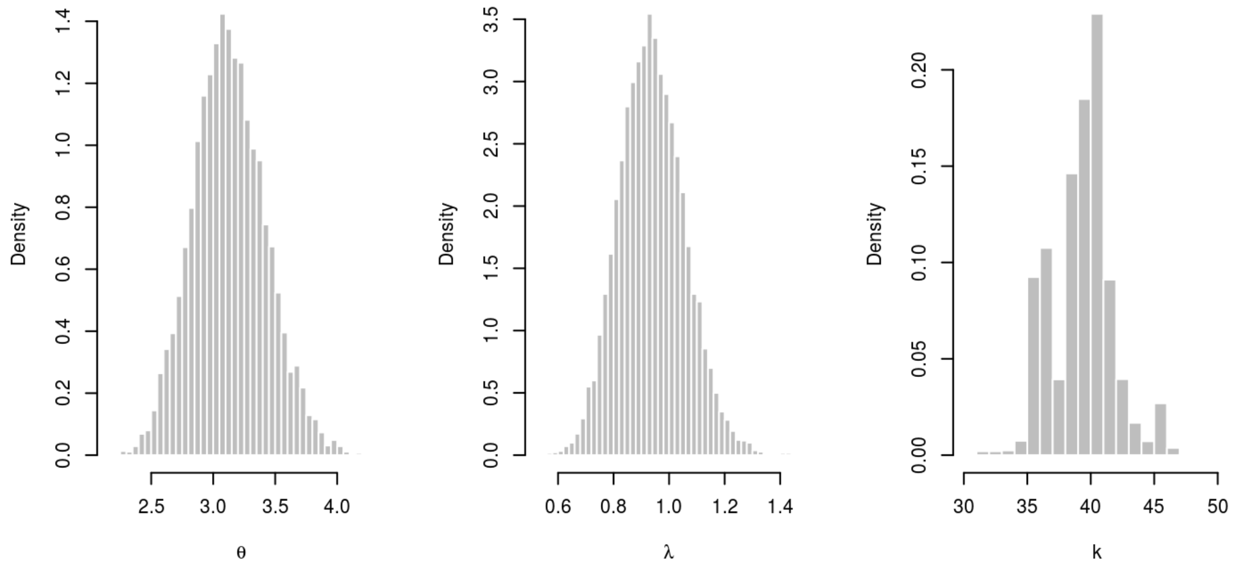
```
print(mean(lambda[burn_in:m])) #[1] 0.9341033
```

```
## [1] 0.939208
```

```
print(mean(theta[burn_in:m])) #[1] 3.108575
```

```
## [1] 3.130795
```

Implementing Gibbs sampling



Our analysis can be used to justify that the change point occurs at some range at the 41^{st} year, 1891, which is similar to other analyses cited by Carlin et al.

Implementing Gibbs sampling

```
hist(theta[burn_in:m], main="", xlab = expression(mu),
     col="gray", border="white",
     breaks = "scott", prob=TRUE) #mu posterior

hist(lambda[burn_in:m], main="", xlab = expression(lambda),
     col="gray", border="white",
     breaks = "scott", prob=TRUE) #lambda posterior

hist(K, breaks=min(K):max(K), prob=TRUE, main="",
     col="gray", border="white",
     xlab = "k")
```

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