Posterior Sampling with MCMC

Andy Shen, Devin Francom

LANL: CCS-6

Overview

Say you have $\mathbf{y}_1, \dots, \mathbf{y}_n \sim N(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ where each $\mathbf{y}_i$ is a vector of length p. Use $n = 100$, $p = 3$, $\boldsymbol{\mu} = (1, 2, 3)$ and

$$\boldsymbol{\Sigma} = \begin{pmatrix} 1.0 & 1.4 & 2.1 \\ 1.4 & 4.0 & 4.2 \\ 2.1 & 4.2 & 9.0 \end{pmatrix}$$

to generate some data

Task 1: Use $\mathbf{y}_1, \dots, \mathbf{y}_n \sim N(\boldsymbol{\mu}, diag(\sigma_1^2, \dots, \sigma_p^2))$ as your likelihood, with $\boldsymbol{\mu} \sim N(\mathbf{m}, \mathbf{S})$ as your prior for $\boldsymbol{\mu}$ and $\sigma_i^2 \sim InvGamma(a, b)$ as your prior for σ_i^2. Use Gibbs sampling to sample the resulting posterior.

Task 2: Now use $\mathbf{y}_1, \dots, \mathbf{y}_n \sim N(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ as your likelihood, with $\boldsymbol{\mu} \sim N(\mathbf{m}, \mathbf{S})$ as your prior for $\boldsymbol{\mu}$ and the diagonal elements of $\boldsymbol{\Sigma}$ as $\sigma_i^2 \sim InvGamma(a, b)$ and each correlation parameter as $\rho_{ij} \sim Beta(a, b)$. Use Gibbs sampling and Metropolis-Hastings to sample the resulting posterior.

Task 1

Our likelihood follows a multivariate normal distribution with mean $\boldsymbol{\mu}$ and variance $diag(\sigma_1^2, \dots, \sigma_p^2)$.

We multiply the likelihood by both priors to get our posterior distribution, $P(\boldsymbol{\mu}, \tilde{\boldsymbol{\Sigma}} \mid \alpha, \beta, \boldsymbol{m}, \boldsymbol{S})$, where $\tilde{\boldsymbol{\Sigma}} = diag(1, 4, 9)$.

We get the following result:

$$P(\boldsymbol{\mu}, \tilde{\boldsymbol{\Sigma}} \mid \alpha, \beta, \boldsymbol{m}, \boldsymbol{S}) \propto exp((\boldsymbol{\mu} - \mathbf{m})' \boldsymbol{S}^{-1} (\boldsymbol{\mu} - \mathbf{m})) \prod_{i=1}^{P=3} \{(\sigma_i^2)^{-\alpha-1} exp(-\frac{\beta}{\sigma_i^2})\} \prod_{i=1}^{100} \{\prod_{j=1}^{3} [\sigma_j^{2^{-1/2}}] exp\{-\frac{1}{2}(\mathbf{y}_i - \boldsymbol{\mu})' \tilde{\boldsymbol{\Sigma}}^{-1} (\mathbf{y}_i - \boldsymbol{\mu})\}\}$$

Our σ_i^2 values follow an inverse gamma distribution with parameters $\alpha + 50$ and $\beta + \frac{1}{2}\sum_{j=1}^{100}(y_{ji} - \mu_i)^2$

$$\sigma_i^2 \sim IG(\alpha + 50, \beta + \frac{1}{2}\sum_{j=1}^{100}(y_{ji} - \mu_i)^2)$$

Our μ_i values follow a univariate normal distribution:

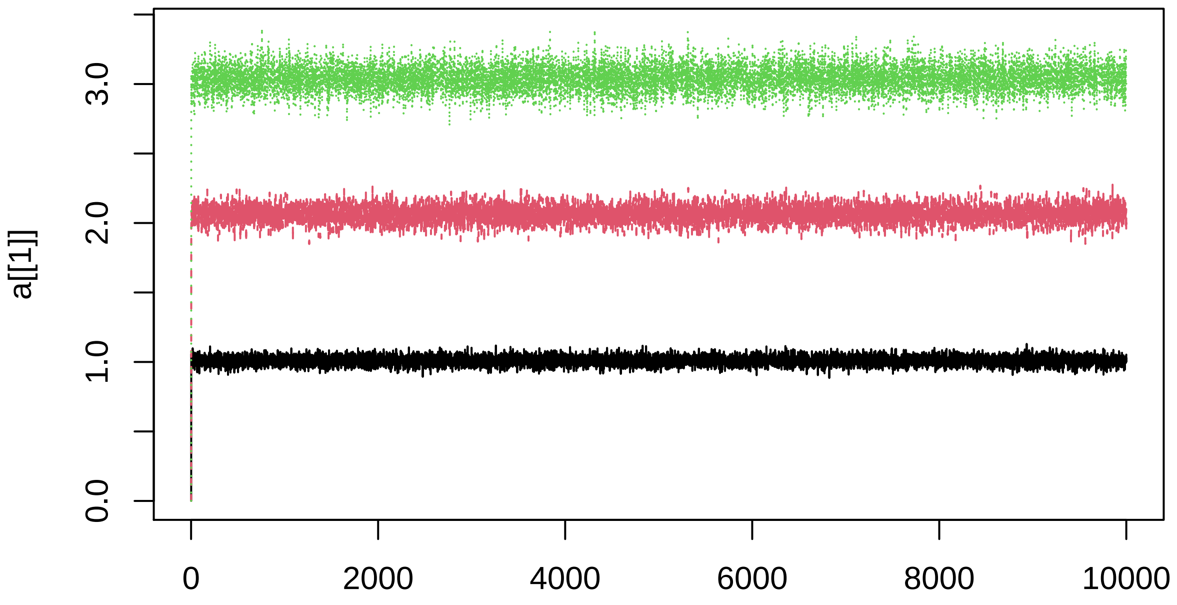
$$\mu_i \sim N(\frac{\sigma_i^2}{\sigma_i^2 + 100 s_i^2} m_i + \frac{s_i^2 \sum_{j=1}^{100} y_j}{\sigma_i^2 + 100 s_i^2}, \frac{\sigma_i^2 s_i^2}{\sigma_i^2 + 100 s_i^2})$$

Posterior Distribution

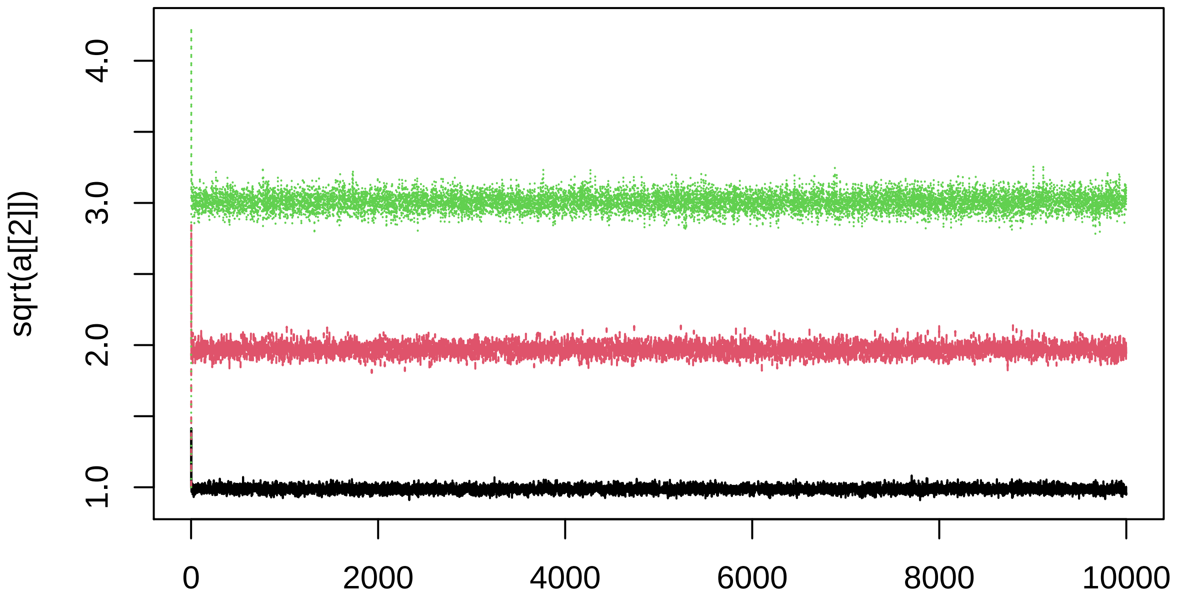
```r
set.seed(123)
library(mvtnorm)
library(invgamma)
mu <- c(1, 2, 3)
sig <- cbind(c(1, 1.4, 2.1), c(1.4, 4.0, 4.2), c(2.1, 4.2, 9.0))
data <- rmvnorm(1000, mu, sig)
n <- nrow(data)
str(data)
```

```
##  num [1:1000, 1:3] 1.234 1.943 0.542 1.295 1.085 ...
```

```r
library(invgamma)
sig_tild <- diag(c(1,4,9))
mu <- mu
S <- diag(3)
M <- c(0,0,0)

## FULL CONDITIONAL DISTRIBUTIONS ##
p_mu <- function(m = M, ST = sig_tild, .S = S, dat = data) {
  sums <- colSums(dat) #update ST
  vals <- rep(NA, 3)
  for(i in seq_len(3)) {
    sig_i <- ST[i,i]
    si <- .S[i,i]
    mi <- m[i]
    mean <- ((sig_i * mi) / (sig_i + n * si)) +
      ((si * sums[i]) / (sig_i + n * si))
    #print(mean)
    var <- (sig_i * si) / (sig_i + n * si)
    vals[i] <- rnorm(1, mean, sqrt(var))
  }
  #return(mean)
  return(vals)
}

p_sig <- function(a = 2, b = 1, dat = data, .mu = mu) {
  centered <- t(t(dat) - .mu) #update .mu
  sums <- colSums(centered^2)
  vals <- rep(NA, 3)
  for(i in seq_len(3)) {
    beta <- 0.5 * sums[i] + b
    vals[i] <- 1/rgamma(1, shape = a + n/2, rate = beta)
  }
  return(vals)
}


gibbs <- function(its = 10000) {
  mat_sig <- matrix(NA, nrow = its, ncol = 3)
  mat_mu <- matrix(NA, nrow = its, ncol = 3)
  mat_sig[1,] <- rep(1, 3)
  mat_mu[1,] <- rep(0, 3)
  for(i in 2:its) {
    # call p_sig with mu = mat_mu[i-1,]
    # call p_mu with updated value from p_sig
    mat_sig[i,] <- p_sig(.mu = mat_mu[i-1,])
    mat_mu[i,] <- p_mu(ST = diag(mat_sig[i,]))
  }
  list(mat_mu, mat_sig)
}
a <- gibbs()
matplot(a[[1]], type = "l")
```



```
matplot(sqrt(a[[2]]), type = "l")
```



Task 2

Our likelihood follows a multivariate normal distribution with mean $\boldsymbol{\mu}$ and variance $diag(\sigma_1^2, \dots, \sigma_p^2)$.

We multiply the likelihood by both priors to get our posterior distribution, $P(\boldsymbol{\mu}, \boldsymbol{\Sigma} \mid \alpha, \beta, \boldsymbol{m}, \boldsymbol{S})$, where

$$\boldsymbol{\mu} = \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix}$$

and

$$\boldsymbol{\Sigma} = \begin{pmatrix} 1.0 & 1.4 & 2.1 \\ 1.4 & 4.0 & 4.2 \\ 2.1 & 4.2 & 9.0 \end{pmatrix}$$

Beta-Gamma-MVN Method

Setting Up Data and Priors

We start by generating the same data from above:

```r
set.seed(123)
library(mvtnorm)
library(invgamma)
mu <- c(1, 2, 3)
sig <- cbind(c(1, 1.4, 2.1), c(1.4, 4.0, 4.2), c(2.1, 4.2, 9.0))
data <- rmvnorm(100, mu, sig)
n <- nrow(data)
str(data)
```

```
##  num [1:100, 1:3] 1.234 1.943 0.542 1.295 1.085 ...
```

```r
S <- diag(3)
Sinv <- solve(S)
m <- c(0,0,0)
```

We have that

$$\boldsymbol{\mu} \mid \cdot \sim \mathcal{N}((\mathbf{S}^{-1} + n\boldsymbol{\Sigma}^{-1})^{-1}(\mathbf{S}^{-1}\boldsymbol{m} + n\boldsymbol{\Sigma}^{-1}\bar{\boldsymbol{y}}), (\mathbf{S}^{-1} + n\boldsymbol{\Sigma}^{-1})^{-1})$$

which is the full conditional distribution for $\boldsymbol{\mu}$.

Recall that for our correlation coefficient ρ_i, we have that

$$\rho_{ij} = \rho_{ji} = \frac{cov(i,j)}{\sigma_i \sigma_j}$$

which we simplify to ρ_i and work with the upper and lower triangular portion of the matrices.

Full Conditionals

```r
p_mu <- function(n = nrow(data), ST) {
  mean <- solve(Sinv + n * solve(ST)) %*% (Sinv %*% m + n * solve(ST) %*% colMeans(data))
  covariance <- solve(Sinv + n * solve(ST))
  rmvnorm(1, mean, covariance)
}

p_sig <- function(alpha = 1, beta = 1, ST, sig_sq, .mu) { # Inverse Gamma Prior
  full_cond <- rep(NA, 3)
  prior <- (-alpha - 1) * log(sig_sq) + (-beta/sig_sq)
  in_sum <- rep(NA, n)
  for(i in seq_len(n)) {
    in_sum[i] <- t(data[i,] - .mu) %*% solve(ST) %*% (data[i,] - .mu)
  }
  sum_all <- -0.5 * sum(in_sum)
  like <- -0.5 * (determinant(ST, logarithm = TRUE)$modulus) + (sum_all)
  full_cond <- prior + like

  (full_cond)
}

p_rho <- function(rho, a = 2, b = 3, .mu, ST) { # Beta Prior
  full_cond <- rep(NA, 3)
  prior <- (a-1) * log(rho) +  (b-1) * log(1-rho)
  in_sum <- rep(NA, n)
  for(i in seq_len(n)) {
    in_sum[i] <- t(data[i,] - .mu) %*% solve(ST) %*% (data[i,] -.mu)
  }
  sum_all <- -0.5 * sum(in_sum)
  like <- -0.5 * (determinant(ST, logarithm = TRUE)$modulus) + (sum_all)
  full_cond <- prior + like

  (full_cond)
}
```

Metropolis-Hastings and Gibbs

```r
set.seed(12)
library(dplyr)
```

```
##
## Attaching package: 'dplyr'

## The following objects are masked from 'package:stats':
##
##     filter, lag

## The following objects are masked from 'package:base':
##
##     intersect, setdiff, setequal, union
```

```r
library(truncnorm)
met_gibbs <- function(its) {

  # For sigma, use truncated normal as proposal
```

```r
propose_sig <- function(x, mean, sd = 1) {
  log(dtruncnorm(x, a = 0, b = 1, mean = mean, sd))
}

propose_rho <- function(x, mean, sd = 1) {
  log(dtruncnorm(x, a = -1, b = 1, mean = mean, sd))
}

met_mu <- matrix(NA, its, 3)
met.mu.start <- rep(0, 3)
met_mu[1,] <- met.mu.start

mat_sig <- matrix(NA, nrow = its, ncol = 3)
mat_rho <- matrix(NA, nrow = its, ncol = 3)
mat_sig[1,] <- rep(1, 3)
mat_rho[1,] <- rep(0, 3) #12, 13, 23
a_sig <- 0
a_rho <- 0
for(i in 2:its) {
  # sample mu with mvn
  #sample sigma given mu
  #sample rho given sigma and mu & rtruncnorm between (-1,1)
  current.mu <- met_mu[i-1,]

  cor_to_cov <- c(
    sqrt(mat_sig[i-1,1] * mat_sig[i-1,2]),
    sqrt(mat_sig[i-1,1] * mat_sig[i-1,3]),
    sqrt(mat_sig[i-1,2] * mat_sig[i-1,3])
  ) #convert correlation to covariance

  cov <- diag(mat_sig[i-1,])
  cov[upper.tri(cov)] <- mat_rho[i-1,] * cor_to_cov
  cov[lower.tri(cov)] <- mat_rho[i-1,] * cor_to_cov
  #browser()
  met_mu[i,] <- p_mu(ST = cov) #Done sampling mu

  ### SIGMA ###

  for(j in 1:3) {
    cov2 <- cov
    candidate_sig <- rtruncnorm(
      1, a = 0, b = 1, mean = met_mu[i,j], sd = 1
    )

    cov2[j,j] <- candidate_sig

    ratio_sig <-
      (p_sig(ST = cov2, sig_sq = cov2[j,j],.mu = met_mu[i,]) -
        propose_sig(candidate_sig, mean = met_mu[i,j], sd = 1) ) -
          (p_sig(ST = cov, sig_sq = cov[j,j], .mu = met_mu[i,]) -
            propose_sig(mat_sig[i-1,j], mean =  met_mu[i,j], sd = 1 ))

    pmove <- min(0, ratio_sig)
```

```r
      if(is.na(pmove)) browser()
      u <- log(runif(1))

      if(u < pmove) {
        mat_sig[i,j] <- candidate_sig
        a_sig = a_sig + 1
        cov <- cov2
      }
      else {
        mat_sig[i,j] <- mat_sig[i-1,j]
      }
    }


    ### RHO ###

    cor_to_cov3 <- c(
      sqrt(mat_sig[i,1] * mat_sig[i,2]),
      sqrt(mat_sig[i,1] * mat_sig[i,3]),
      sqrt(mat_sig[i,2] * mat_sig[i,3])
    ) #convert correlation to covariance



    for(k in 1:3) {
      candidate_rho <- rtruncnorm(
      1, a = 0, b = 1, mean = met_mu[i,k], sd = 1
      )

      cov3 <- cov
      cov3[upper.tri(cov3)] <- candidate_rho * cor_to_cov3
      cov3[lower.tri(cov3)] <- candidate_rho * cor_to_cov3
      ratio_cov <-
      (p_rho(rho = candidate_rho, .mu = met_mu[i,], ST = cov3) -
        propose_rho(candidate_rho, mean = met_mu[i,k], sd = 1)) -
        (p_rho(rho=cov3[upper.tri(cov3)][k]/cor_to_cov3[k], .mu = met_mu[i,], ST = cov2) -
          propose_rho(mat_rho[i-1,k], mean = met_mu[i,k], sd = 1))
      #browser()
      pmove <- min(0, ratio_cov)
      #if(is.na(pmove)) browser()
      u <- log(runif(1))
      if(u < pmove) {
        #if(is.na(candidate_rho)) browser()
        mat_rho[i,k] <- candidate_rho
        a_rho = a_rho + 1
        cov <- cov3
      }
      else {
        mat_rho[i,k] <- mat_rho[i-1,k]
      }
    }
  }
  list(met_mu, mat_sig, mat_rho, a_sig, a_rho)
```

```r
}

its <- 1000
a <- met_gibbs(its = its)
```

```r
tail(a[[1]])
```

```
##              [,1]     [,2]     [,3]
##  [995,] 0.9236514 1.857613 2.960463
##  [996,] 0.9996535 2.020661 3.094557
##  [997,] 1.0459543 1.859307 3.043632
##  [998,] 0.9744608 1.955628 3.044519
##  [999,] 1.1476173 1.995296 3.181229
## [1000,] 1.0119333 1.925337 3.054327
```

```r
colMeans(a[[1]])
```

```
## [1] 1.029623 1.967629 3.085902
```

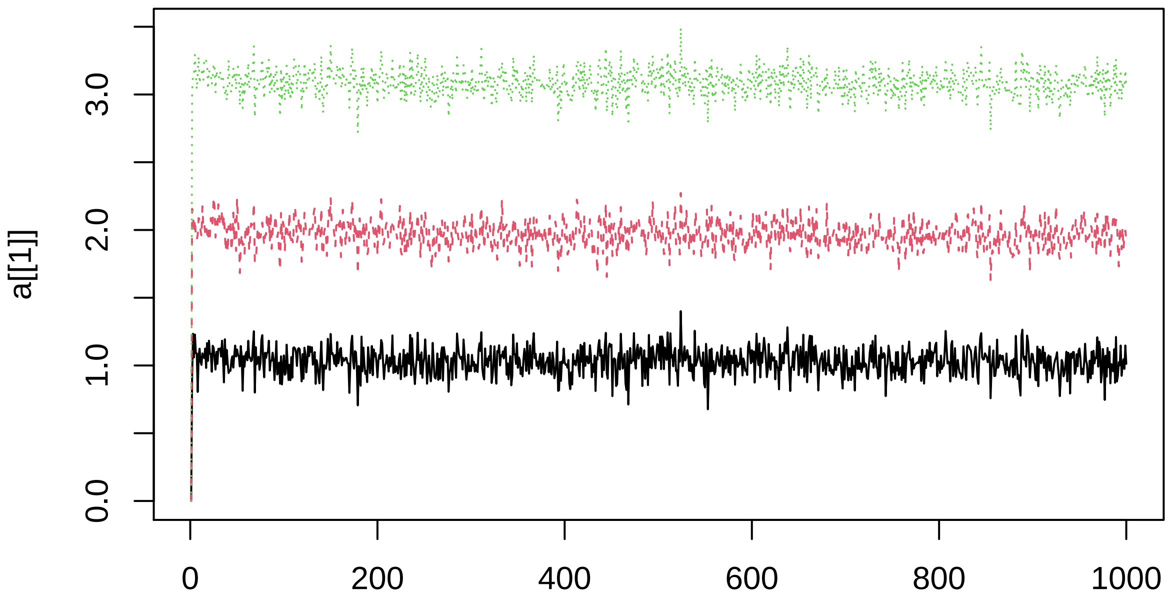
```r
colMeans(a[[2]])
```

```
## [1] 0.9780484 0.9877242 0.9876616
```

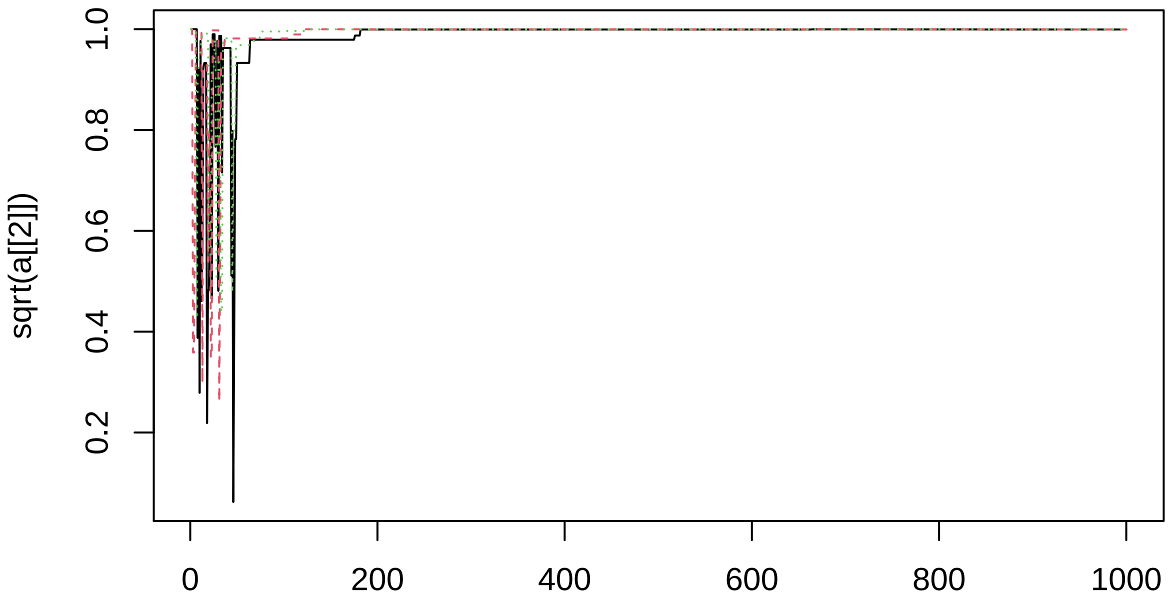
```r
colMeans(a[[3]])
```

```
## [1] 0.4698454 0.9671691 0.8624496
```

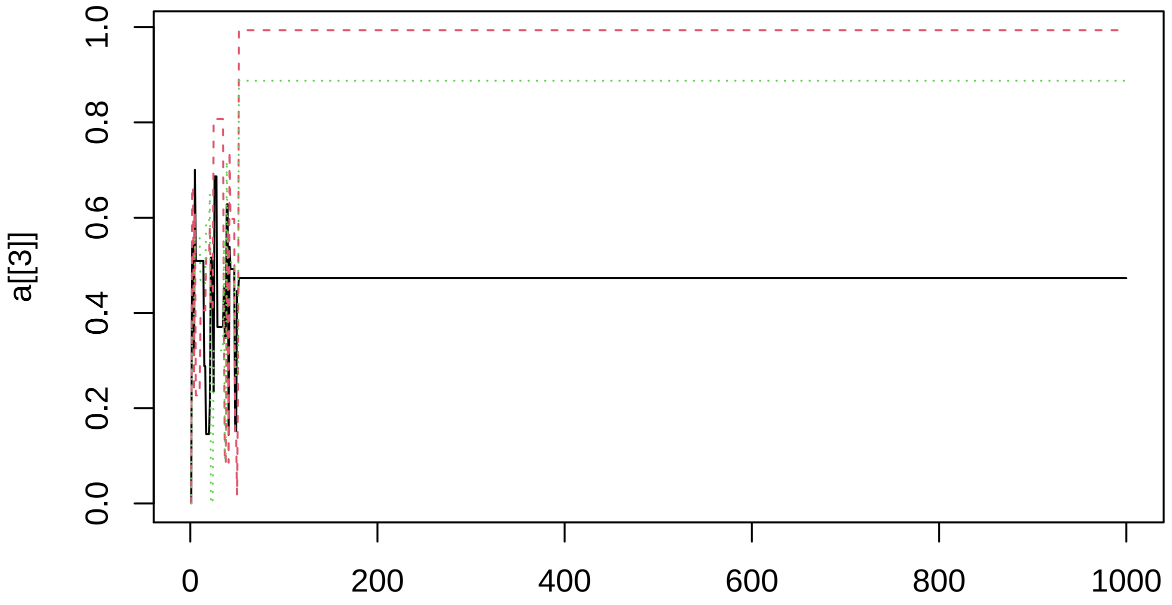
```r
matplot(a[[1]], type = "l")
```



```r
matplot(sqrt(a[[2]]), type = "l")
```



```
matplot(a[[3]], type = "l")
```



```
sig <- 1:3
rho <- 4:6
lol <- 4:6
mat <- diag(sig)
mat[upper.tri(mat)] <- rho
 mat[lower.tri(mat)] <- lol
mat
```

```
##      [,1] [,2] [,3]
## [1,]    1    4    5
## [2,]    4    2    6
## [3,]    5    6    3
```

```
mat2 <- mat
o <- rnorm(3); o
```

```
## [1] -0.3329931 -0.1453455  0.2614401
```

```
for(i in 1:nrow(mat)) {
  mat2[i,i] <- o[i]
}
mat2[1,] * c(1,0, 10)
```

```
## [1] -0.3329931  0.0000000 50.0000000
```

Inverse-Wishart Method

We will largely use the precision matrix, Λ which is simply just $\mathbf{\Sigma}^{-1}$.

In our case, we have that

$$\mathbf{\Lambda} = \begin{pmatrix} 2.361 & -0.486 & 0.324 \\ -0.486 & 0.590 & -0.162 \\ -0.324 & -0.162 & 0.262 \end{pmatrix}$$

It then follows that

$$\mathbf{y_i} \mid \boldsymbol{\mu}, \mathbf{\Lambda} \sim \mathcal{N}(\boldsymbol{\mu}, \mathbf{\Lambda}^{-1})$$

$$\mathbf{\Lambda} \sim W(\mathbf{S}, n_0)$$

From this intuition, and leveraging the fact that $\mathbf{\Lambda} = \mathbf{\Sigma}^{-1}$, it then follows the full conditional of our covariance matrix $\mathbf{\Sigma}$ follows an Inverse Wishart Distribution:

$$\mathbf{\Sigma} \sim W^{-1}(\mathbf{S}^{-1} + \sum_{j=1}^{100} (\boldsymbol{y}_j - \boldsymbol{\mu})(\boldsymbol{y}_j - \boldsymbol{\mu})', n_0 + n)$$

where n_0 represents the degrees of freedom such that $n_0 = p - 1$ where $p = dim(S)$, where S is a positive-definite matrix.

The Algorithms

```
mu <- mu
S <- diag(3)
Sinv <- solve(S)
M <- c(0,0,0)
Lam <- solve(sig); Lam
```

```
## Error in solve.default(sig): 'a' (3 x 1) must be square
```

```
## Error in eval(expr, envir, enclos): object 'Lam' not found
```

```
p <- dim(sig)[1]
```

```
library(MCMCpack)
```

```
## Loading required package: coda
## Loading required package: MASS
##
## Attaching package: 'MASS'
## The following object is masked from 'package:dplyr':
##
##     select
## ##
## ## Markov Chain Monte Carlo Package (MCMCpack)
## ## Copyright (C) 2003-2020 Andrew D. Martin, Kevin M. Quinn, and Jong Hee Park
## ##
## ## Support provided by the U.S. National Science Foundation
## ## (Grants SES-0350646 and SES-0350613)
## ##
##
## Attaching package: 'MCMCpack'
## The following objects are masked from 'package:invgamma':
##
##     dinvgamma, rinvgamma
```

```
p_muvec <- function(n = nrow(data)) {
  mean <- solve(Sinv + n * Lam) %*% (Sinv %*% M + n * Lam %*% colMeans(data))
  cov <- solve(Sinv + n * Lam)
  rmvnorm(1, mean, cov)
}

p_cov <- function(mu, df = p, n = nrow(data)) {
  summation <-
  pdmat <- Sinv + summation
  riwish(df + n, pdmat)
}

gibbs <- function(its = 10) {
  mat_sig <- array(NA, dim = c(3, 3, its))
  mat_mu <- matrix(NA, nrow = its, ncol = 3)
  mat_sig[1,1,1] <- diag(3)
  mat_mu[1,] <- rep(0, 3)
  for(i in 2:its) {
    # call p_sig with mu = mat_mu[i-1,]
    # call p_mu with updated value from p_sig
    mat_sig[i,] <- p_cov()
    mat_mu[i,] <- p_mu(ST = diag(mat_sig[i,]))
  }
  list(mat_mu, mat_sig)
}
```

```
a <- array(NA, c(2,2,5))
select_ar <- matrix(ncol = 2, byrow = TRUE, c(
1,2,
2,1))
a[1:2,1:2,1:3]
```

```
## , , 1
##
##      [,1] [,2]
## [1,]   NA   NA
## [2,]   NA   NA
##
## , , 2
##
##      [,1] [,2]
## [1,]   NA   NA
## [2,]   NA   NA
##
## , , 3
##
##      [,1] [,2]
## [1,]   NA   NA
## [2,]   NA   NA
```