

Exercise 1: Let the discrete random variable X be described by a probability mass function $p_X(x) = \Pr(X = x)$. The current state of a Metropolis–Hastings Markov chain is x_t , which is generated from the same distribution as X. Demonstrate that the next state x_{t+1} will also be drawn from the same distribution as X.

Solution: Let's assume the following labels for the states of the Markov chain: $x_{t+1} = x_b$ and $x_t = x_a$. The Metropolis–Hastings ratio is

$$r(x_b | x_a) = \frac{q(x_a | x_b)p(x_b)}{q(x_b | x_a)p(x_a)}.$$

The joint probability that $X_{t+1} = x_b$ and $X_t = x_a$ can be decomposed as

$$\Pr(X_{t+1} = x_b, X_t = x_a) = \Pr(X_{t+1} = x_b | X_t = x_a) \Pr(X_t = x_a).$$

The Markov chain reaches state x_b at time t+1 if this state is proposed and accepted. Let's assume that $r(x_b | x_a) > 1$ and consequently $r(x_a | x_b) < 1$ so that

$$\Pr(X_{t+1} = x_b, X_t = x_a) = \min[1, r(x_b \mid x_a)]q(x_b \mid x_a)\Pr(X_t = x_a) = q(x_b \mid x_a)p(x_a)$$

On the other hand,

$$Pr(X_{t+1} = x_a, X_t = x_b) = Pr(X_{t+1} = x_a | X_t = x_b)Pr(X_t = x_b)$$
$$= \min[1, r(x_a | x_b)]q(x_a | x_b)p(x_b)$$
$$= \frac{q(x_b | x_a)p(x_a)}{q(x_a | x_b)p(x_b)}q(x_a | x_b)p(x_b)$$
$$= q(x_b | x_a)p(x_a)$$
$$= Pr(X_{t+1} = x_b, X_t = x_a)$$

implying that $\Pr(X_{t+1} = x_b, X_t = x_a) = \Pr(X_{t+1} = x_a, X_t = x_b)$. Marginalization of the joint distribution shows that $\Pr(X_{t+1} = x_b) = \Pr(X_t = x_b)$ and since X_t follows the same distribution as X, the next random variable X_{t+1} follows that distribution as well.

Exercise 2 (chapter 7.4): Let the random variable X follow a Laplace distribution with location $\mu = 0$ and scale parameter $\sigma = 2$. The density of the Laplace distribution is

$$f_X(x) = \frac{1}{2\sigma} \exp\left\{-\frac{|x-\mu|}{\sigma}\right\} \qquad \sigma > 0.$$

- 1. Implement an independent Metropolis–Hastings sampler with a Normal $(0, \sigma_1^2)$ proposal distribution.
- 2. Implement a random walk Metropolis–Hastings sampler based on Normal $(0, \sigma_2^2)$ noise.

3. Compare the performance of both samplers in terms of $\mathbb{E}[X]$ and $\mathbb{V}[X]$ for various values of σ_1^2 and σ_2^2 . What value of σ_2^2 is required to achieve an acceptance rate of about 40% in case of the random walk Metropolis-Hastings sampler?

Solution: An implementation of the independent Metropolis-Hastings sampler in R is:

```
target <- function(x) { -0.5 * abs(x) }
proposal <- function( x, scale ) { dnorm( x, 0, scale, TRUE ) }</pre>
nSamples <- 10000 ; nAccepted <- 0
x <- numeric( nSamples ) ; sigma1 <- 6;</pre>
for( ii in seq( 2, nSamples ) ) {
   x[ ii ] <- rnorm( 1, 0, sigma1 )
   alpha <- exp(
      proposal( x[ ii - 1 ], sigma1 ) + target( x[ ii ] ) -
      proposal( x[ ii ], sigma1 ) - target( x[ ii - 1 ] )
   )
   if( runif( 1 ) > alpha ) {
      x[ ii ] <- x[ ii - 1 ]
   } else {
      nAccepted <- nAccepted + 1
   }
}
```

An implementation of the random walk Metropolis–Hastings sampler in R is:

```
target <- function( x ) { -0.5 * abs( x ) }
nSamples <- 10000 ; nAccepted <- 0
x <- numeric( nSamples ) ; sigma2 <- 6
for( ii in seq( 2, nSamples ) ) {
    x[ ii ] <- rnorm( 1, x[ ii - 1 ], sigma2 )
    alpha <- exp( target( x[ ii ] ) - target( x[ ii - 1 ] ) )
    if( runif( 1 ) > alpha ) {
        x[ ii ] <- x[ ii - 1 ]
    } else {
        nAccepted <- nAccepted + 1
    }
}</pre>
```

A comparison of both samplers for different values of σ_1^2 and σ_2^2 is shown below. In case of the random walk Metropolis–Hastings sampler, the acceptance rate is high for small values of σ_2^2 (first trace plot). Successive states of the Markov chain are very similar which results in a slow exploration of the distribution and convergence to it. If σ_2^2 is too large (second trace plot), then the proposed states are likely in regions with low probability density which also results in a slow exploration of the distribution and convergence to it.

The value of σ_2^2 has to be between 25 and 100 to achieve an acceptance rate of about 40%. Since $\mathbb{V}[X] = 8$, $\sigma_2^2 = 2.38^2 \cdot 8 \approx 45$ (chapter 7.4.3) results in an acceptance rate of about 40%.





Exercise 3 (chapter 7.4): Let $\{Y_i\}_{i=1}^3$ be independent and identically distributed random variables that follow a Cauchy distribution with location μ and scale parameter $\sigma = 1$. The density of the Cauchy distribution is

$$f_Y(y) = \frac{1}{\pi} \left[\frac{\sigma}{\sigma^2 + (y - \mu)^2} \right] \qquad \sigma > 0$$

The prior density of the location parameter is $p(\mu) \propto \exp\{-\mu^2/100\}$.

- 1. Show that the posterior density has three modes when $Y_1 = 0, Y_2 = 5$ and $Y_3 = 9$.
- 2. Implement a random walk Metropolis–Hastings sampler based on Cauchy $(0, \sigma_1^2)$ and Normal $(0, \sigma_2^2)$ noise.
- 3. Compare the performance of both samplers in terms of $\mathbb{E}[\mu | y_1, y_2, y_2]$ and monitor convergence using cumulative average plots.

Solution: Trimodality could be checked visually.



An implementation of both random walk Metropolis–Hastings samplers in R is:

```
target <- function( mu, y ) {</pre>
   -mu ^ 2 / 100 -
  log(1 + (y[1] - mu)^2) -
  log(1 + (y[2] - mu)^2) -
   log(1 + (y[3] - mu)^2)
}
nSamples <- 10000 ;
x <- matrix( 0, nSamples, 2 ) ; y <- c( 0, 5, 9 ) ; sigma <- 0.01
for( ii in seq( 2, nSamples ) ) {
  x[ ii, 1 ] <- rnorm( 1, x[ ii - 1, 1 ], sigma )
   x[ ii, 2 ] <- rcauchy( 1, x[ ii - 1, 2 ], sigma )
   alpha <- c(
      exp( target( x[ ii, 1 ], y ) - target( x[ ii - 1, 1 ], y ) ),
      exp( target( x[ ii, 2 ], y ) - target( x[ ii - 1, 2 ], y ) )
   )
   if( runif( 1 ) > alpha[ 1 ] ) {
      x[ii, 1] <- x[ii - 1, 1]
   }
   if( runif( 1 ) > alpha[ 2 ] ) {
      x[ii, 2] <- x[ii - 1, 2]
   }
}
```

Cauchy noise works well in terms of convergence and posterior mean estimation regardless of the value of σ_1^2 . Conversely, normal noise only works for $\sigma_2^2 = 10$. For $\sigma_2^2 = 0.01$ and $\sigma_2^2 = 0.5$, convergence does not occur during the number of iterations or posterior mean approximation is too biased.



Exercise 4: Let X and Y be discrete random variables with support $\{x_1, \ldots, x_n\}$ and $\{y_1, \ldots, y_m\}$. Denote the joint probability mass function of X and Y by $p_{X,Y}(x,y) = \Pr(X = x, Y = y)$. Using a Gibbs sampler, assume that convergence to the distribution of (X, Y) has occurred. Demonstrate that the next state (x_{t+1}, y_{t+1}) will also be drawn from the same distribution as (X, Y).

Solution: By the law of total probability,

$$\Pr(X_{t+1} = x_{t+1}, Y_{t+1} = y_{t+1}) = \sum_{i,j} \left[\Pr(X_{t+1} = x_{t+1}, Y_{t+1} = y_{t+1} | X_t = x_i, Y_t = y_j) \right]$$
$$\Pr(X_t = x_i, Y_t = y_j) \right].$$

Assume that the next state (x_{t+1}, y_{t+1}) is generated by first drawing from the conditional distribution Y | X and subsequently from X | Y. In that case

$$\begin{aligned} \Pr(X_{t+1} = x_{t+1}, Y_{t+1} = y_{t+1} \mid X_t = x_i, Y_t = y_j) &= \Pr(X_{t+1} = x_{t+1} \mid Y_{t+1} = y_{t+1}) \times \\ \Pr(Y_{t+1} = y_{t+1} \mid X_t = x_i) \,. \end{aligned}$$

The joint probability that $X_{t+1} = x_{t+1}$ and $Y_{t+1} = y_{t+1}$ is therefore

$$\begin{aligned} \Pr(X_{t+1} = x_{t+1}, Y_{t+1} = y_{t+1}) &= \Pr(X_{t+1} = x_{t+1} \mid Y_{t+1} = y_{t+1}) \times \\ &\sum_{i,j} \Pr(Y_{t+1} = y_{t+1} \mid X_t = x_i) \Pr(X_t = x_i, Y_t = y_j) \\ &= \frac{p(x_{t+1}, y_{t+1})}{p(y_{t+1})} \sum_{i,j} \frac{p(x_i, y_{t+1})}{p(x_i)} p(y_j \mid x_i) p(x_i) \\ &= \frac{p(x_{t+1}, y_{t+1})}{p(y_{t+1})} \sum_i p(x_i, y_{t+1}) \sum_j p(y_j \mid x_i) \\ &= p(x_{t+1}, y_{t+1}), \end{aligned}$$

which shows that (X_{t+1}, Y_{t+1}) follows the same distribution as (X, Y).

Exercise 5 (chapter 7.5): Let the vector $\boldsymbol{X} = [X_1, X_2]^{\mathrm{T}}$ follow a bivariate Normal distribution with

zero mean vector and covariance matrix $\begin{bmatrix} 1 & \rho \\ \rho & 1 \end{bmatrix}$ with $|\rho| < 1$.

- 1. Implement Monte Carlo simulation and Gibbs sampling to compute marginal expectations and variances.
- 2. Use $\rho = 0$ and generate 500 samples. Compare both methods in terms of bias.
- 3. Use $\rho = 0.5, 0.9, 0.99, 0.999$ and generate again 500 samples. Create trace plots and explain how the correlation affects Gibbs sampling.
- 4. Repeat 2. and 3. by generating 10 000 samples. Explain how Gibbs sampling improves in terms of bias when generating more samples.

Solution: The conditional density of X_1 given $X_2 = x_2$ is

$$\begin{split} f_{X_1|X_2}(x_1 \mid x_2) &= \frac{f_{X_1,X_2}(x_1,x_2)}{f_{X_2}(x_2)} \\ &= \frac{1}{2\pi\sqrt{1-\rho^2}} \exp\left\{-\frac{x_1^2 - 2\rho x_1 x_2 + x_2^2}{2(1-\rho^2)}\right\} \middle/ \frac{1}{\sqrt{2\pi}} \exp\left\{-\frac{x_2^2}{2}\right\}, \\ &= \frac{1}{\sqrt{2\pi(1-\rho^2)}} \exp\left\{-\frac{(x_1 - \rho x_2)^2}{2(1-\rho^2)}\right\} \end{split}$$

which can be recognized as the density of a Normal $(\rho x_2, 1 - \rho^2)$ distribution. Inversely, the conditional distribution of X_2 given $X_1 = x_1$ is Normal $(\rho x_1, 1 - \rho^2)$. An implementation of Monte Carlo simulation and Gibbs sampling in R is:

```
rho <- 0.5 ; Sigma <- matrix( c( 1, rho, rho, 1 ), 2, 2 ) ;
scale <- sqrt( 1 - rho ^ 2 ) ; nSamples <- 10000 ;
x <- array( 0, c( nSamples, 2, 2 ) )
x[, , 1 ] <- mvtnorm::rmvnorm( nSamples, sigma = Sigma )
for( ii in seq( 2, nSamples ) ) {
    x[ ii, 1, 2 ] <- rnorm( 1, rho * x[ ii - 1, 2, 2 ], scale )
    x[ ii, 2, 2 ] <- rnorm( 1, rho * x[ ii - 1, 1, 2 ], scale )
}</pre>
```

For $\rho = 0$ and 500 samples, the performance of both methods in terms of bias is:

Expectations (MC): -0.01832 0.08145
Expectations (Gibbs): -0.00554 0.06355
Variances (MC): -0.06087 -0.07836
Variances (Gibbs): 0.02799 0.07053

Monte Carlo simulation and Gibbs sampling are equivalent for $\rho = 0$, because the conditional distributions reduce to marginals and generating from the bivariate distribution is equivalent to drawing from the marginals due to independence. For $\rho = 0.5, 0.9, 0.99, 0.999$, the performance of both methods is:





For $\rho = 0$ and 10000 samples, the performance of both methods in terms of bias is:

```
# Expectations (MC): 0.0122 0.007333
```

Expectations (Gibbs): -0.01249 -0.006557

Variances (MC): -0.01316 0.008621

```
# Variances (Gibbs): 0.01814 0.008486
```

For $\rho = 0.5, 0.9, 0.99, 0.999$, the performance of both methods is:

#		E[X1]	(MC)	E[X2]	(MC)	Var[X1]] (MC)	Var[X2]	(MC)	
#	0.5	0.00)1906	-0.00	04195		1.001	0.9	9984	
#	0.9	-0.00)3444	-0.00	01229		1.004	1.0	0026	
#	0.99	-0.00	9029	-0.00	08474		1.003	1.0	0048	
#	0.999	0.00)2127	0.00	01981		1.008	1.0	0089	
#		E[X1]	(Gibl	bs) E[2	(2] (0	Gibbs) '	Var[X1]] (Gibbs)	Var[X2]	(Gibbs)
#	0.5	(0.0028	319	0.0	001682		1.0080		1.0056
#	0.9	(0.013	091	0.0	012947		1.0093		1.0095
#	0.99	().0556	644	0.0	055629		1.0287		1.0289
#	0.999	-0).2342	236	-0.2	234031		0.7897		0.7898



The performance of both methods increases with the number of generated draws. However, for very large values of ρ , Gibbs sampling is still very biased and convergence diagnostics are necessary.

Exercise 6 (chapter 7.5): Let $\{y\}_{i=1}^{n}$ be observations from a counting process where

$$y_i \mid \mu_1, \mu_2, \lambda \sim \begin{cases} \text{Poisson}(\mu_1) & \text{if } i \leq \lambda \\ \text{Poisson}(\mu_2) & \text{if } i > \lambda \end{cases}$$

and λ denotes a change point. Let the priors be

$$\mu_1 \sim \text{Gamma}(\alpha_1, \beta_1)$$
$$\mu_2 \sim \text{Gamma}(\alpha_2, \beta_2) \qquad .$$
$$\lambda \sim \text{Uniform}(1, 2, \dots, n)$$

- 1. Find the likelihood and joint posterior density for the changepoint model.
- 2. Find all full conditional densities to implement a Gibb sampler.
- 3. Use the Gibbs sampler and the following data to perform changepoint detection:

 $\begin{array}{l}4,4,3,1,3,2,1,0,11,11,12,4,4,7,9,6,9,12,13,15,12,10,10,6,6,7,12,11,\\15,5,11,8,11,7,11,12,14,12,8,11,9,10,6,14,14,8,4,7,10,3,14,10,17,7,\\16,9,12,11,7,11,5,11,13,9,7,9,7,11,12,13,6,9,10,13,8,18,6,16,8,4,16,\\8,9,5,7,9,10,11,13,12,9,11,7,9,6,7,6,11,8,5\end{array}$

Solution: The likelihood and posterior density are

$$p(\mu_1, \mu_2, \lambda \mid y) \propto p(y \mid \mu_1, \mu_2, \lambda) p(\mu_1) p(\mu_2) p(\lambda)$$

= $\left[\prod_{i=1}^{\lambda} \mu_1^{y_i} \exp\{-\mu_1\} \prod_{i=\lambda+1}^{n} \mu_2^{y_i} \exp\{-\mu_2\}\right] \left[\mu_1^{\alpha_1 - 1} \exp\{-\beta_1 \mu_1\}\right] \left[\mu_2^{\alpha_2 - 1} \exp\{-\beta_2 \mu_2\}\right]$

The full conditional density of μ_1 is

$$p(\mu_1 \mid \mu_2, \lambda, y) \propto \prod_{i=1}^{\lambda} \mu_1^{y_i} \exp\{-\mu_1\} \mu_1^{\alpha_1 - 1} \exp\{-\beta_1 \mu_1\}$$
$$= \mu_1^{\alpha_1 + (\sum_{i=1}^{\lambda} y_i) - 1} \exp\{-\mu_1(\beta_1 + \lambda)\},$$

which can be recognized as the density of a $\operatorname{Gamma}\left(\alpha_1 + \sum_{i=1}^{\lambda} y_i, \beta_1 + \lambda\right)$ distribution. The full conditional density of μ_2 is

$$p(\mu_2 \mid \mu_1, \lambda, y) \propto \prod_{i=\lambda+1}^n \mu_2^{y_i} \exp\{-\mu_2\} \mu_2^{\alpha_2 - 1} \exp\{-\beta_2 \mu_2\}$$
$$= \mu_2^{\alpha_2 + (\sum_{i=\lambda+1}^n y_i) - 1} \exp\{-\mu_2(\beta_2 + n - \lambda)\},$$

which can be recognized as the density of a $\operatorname{Gamma}(\alpha_2 + \sum_{i=\lambda+1}^n y_i, \beta_2 + n - \lambda)$ distribution. The full conditional (probability mass function) of λ is

$$p(\lambda \mid \mu_1, \mu_2, y) \propto \prod_{i=1}^{\lambda} \mu_1^{y_i} \exp\{-\mu_1\} \prod_{i=\lambda+1}^{n} \mu_2^{y_i} \exp\{-\mu_2\} \qquad \lambda = 1, 2, \dots, n$$

An implementation of Monte Carlo simulation and Gibbs sampling in R is:

```
a1 <- b1 <- a2 <- b2 <- 1
n <- length( y ) ; nSamples <- 2000</pre>
x <- matrix( 0, nSamples, 3 ) ; x[ 1, 3 ] <- 10
grid <- seq_len( n )</pre>
for( ii in seq( 2, nSamples ) ) {
   x[ ii, 1 ] <- rgamma(
      1,
      a1 + sum( y[ 1 : x[ ii - 1, 3 ] ]),
      b1 + x[ ii - 1, 3 ]
   )
   x[ ii, 2 ] <- rgamma(
      1,
      a2 + sum( y[ ( x[ ii - 1, 3 ] + 1 ) : n ] ),
      b2 + n - x[ii - 1, 3]
   )
   like1 <- cumsum( dpois( y[ grid ], x[ ii, 1 ], TRUE ) )</pre>
   like2 <- dpois( y[ grid[ -1 ] ], x[ ii, 2 ], TRUE )</pre>
   like2 <- sapply( 1 : length( like2 ), function( ii, nLike2 ) {</pre>
      sum( like2[ ii : nLike2 ] ), nLike2 = length( like2 )
   })
   probs <- like1 + c( like2, 0 )</pre>
   maxProb <- max( probs )</pre>
```

sumProbs <- maxProb + log(sum(exp(probs - maxProb)))
probs <- exp(probs - sumProbs)
x[ii, 3] <- sample(grid , 1, FALSE, probs)</pre>

Gibbs sampling using 10 000 draws resulted the following posterior mean estimates for the above data:

```
# mu1 mu2 lambda
# 2.110 9.524 8.000
```

}

The true parameter values are $\mu_1 = 2$, $\mu_2 = 10$ and $\lambda = 8$.

Exercise 7 (chapter 7.8): Let $\{X_i\}_{i=1}^n$ be correlated random variables with $\mathbb{V}[X_i] = \sigma^2$ for all i = 1, ..., n and $\operatorname{Cov}[X_i, X_{i+k}] = \sigma_k$ for all i, k. Consider the sample mean $\overline{X} = n^{-1} \sum_{i=1}^n X_i$ and find its variance $\mathbb{V}[\overline{X}]$.

Solution: The variance of the sample mean is

$$\mathbb{V}[\bar{X}] = \mathbb{V}\left[\frac{1}{n}\sum_{i=1}^{n}X_{i}\right]$$

= $\frac{1}{n^{2}}\mathbb{V}[X_{1} + (X_{2} + \ldots + X_{n})]$
= $\frac{1}{n^{2}}(\mathbb{V}[X_{1}] + 2\mathrm{Cov}[X_{1}, X_{2} + \ldots + X_{n}] + \mathbb{V}[X_{2} + \ldots + X_{n}])$
= $\frac{1}{n^{2}}(\sigma^{2} + 2[\sigma_{1} + \ldots + \sigma_{n-1}] + \mathbb{V}[X_{2} + \ldots + X_{n}])$

Continuing in a similar manner with $\mathbb{V}[X_2 + \ldots + X_n]$ and all subsequent variances yields

$$\mathbb{V}\left[\bar{X}\right] = \frac{1}{n^2} \left(n\sigma^2 + 2\left[(n-1)\sigma_1 + \ldots + \sigma_{n-1}\right]\right)$$
$$= \frac{\sigma^2}{n} \left(1 + 2\left[\frac{(n-1)\sigma_1}{n\sigma^2} + \ldots + \frac{\sigma_{n-1}}{n\sigma^2}\right]\right)$$
$$= \frac{\sigma^2}{n} \left(1 + 2\sum_{j=1}^{n-1} \left[\frac{n-j}{n}\right] \frac{\sigma_j}{\sigma^2}\right)$$
$$= \frac{\sigma^2}{n} \left(1 + 2\sum_{j=1}^{n-1} \left[1 - \frac{j}{n}\right]\rho_j\right)$$

where $\rho_j = \sigma_j / \sigma^2$ is the correlation at lag j, that is, the correlation between X_i and X_{i+k} . Note that the variance of the sample mean can be used in MCMC sampling to compute numerical standard errors. These numerical standard errors help quantify the uncertainty on $\mathbb{E}[h(\theta)]$ due to MCMC sampling. It can also be used to determine the number of MCMC draws as it tends to 0 with increasing draws.