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Bayesian Statistics

Markov Chain Monte Carlo methods Leonardo Egidi

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A partial change of paradigm

Up to now we have typically generated iid variables directly from the density of interest π or indirectly in the case of importance sampling.

The Metropolis-Hastings algorithm and the Gibbs sampling generate instead *correlated* variables from a stochastic process called Markov chain. Markov chains carry different convergence properties that can be exploited to provide easier proposals in cases where generic importance sampling does not readily apply.

We will briefly review these stochastic process to fully understand how an MCMC algorithm works and to program it in a proper way.

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The basic problem

Suppose we want to draw from our posterior distribution $\pi(\theta|y)$, but we cannot sample independent draws from it. For example, we often do not know the normalizing constant.

However, we may be able to sample draws from $\pi(\theta|y)$ that are slightly dependent. If we can sample slightly dependent draws using a Markov chain, then we can still find quantities of interests from those draws.

This process is called Monte Carlo Integration. Basically a fancy way of saying we can take quantities of interest of a distribution from simulated draws from the distribution.

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Stochastic process

Def (Stochastic process)

Given a state space Ω and a sequence of consecutive time instants $\mathcal{T} = [0,T]$, a stochastic process $\{X^{(t)}\}_{t \in \mathcal{T}}$ is defined as a collection of random variables, i.e., each $X^{(t)}: \Omega \to E$ is a measurable function from the set of possible outcomes Ω to a measurable space E.

Informally, a stochastic process is then a consecutive set of random quantities defined on some known state space.

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Notation In the Bayesian framework, we use the symbol θ to refer to the random parameter(s), and we will consider a draw of $\theta^{(s)}$ to be the state of the chain at iteration $s, s = 1, \ldots, S$, where S is the total number of desired simulations.

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Markov chains

A Markov chain is a stochastic process in which future states are independent of past states given the present state.

Def (Markov chain)

A Markov chain $\{X^{(t)}\}$ is a sequence of dependent random variables

$$X^{(0)}, X^{(1)}, \ldots, X^{(t)}, \ldots$$

such that the probability distribution of $X^{(t)}$ given the past variables depends only on the last value, $X^{(t-1)}$. This conditional probability distribution is called a transition kernel K, that is:

$$X^{(t)}|X^{(0)},X^{(1)},\ldots,X^{(t-1)}\sim K(X^{(t-1)},X^{(t)}).$$

In other words, $p(X^{(t)}|X^{(0)},X^{(1)},\ldots,X^{(t-1)}) \equiv p(X^{(t)}|X^{(t-1)}).$

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Examples of Markov chains

Examples:

1 a simple random walk stochastic process satisfies:

$$X^{(t+1)} = X^{(t)} + \epsilon_t, \tag{1}$$

where $\epsilon_t \sim \mathcal{N}(0,1)$, independently of $X^{(t)}$; therefore, the Markov kernel $K(X^{(t)},X^{(t+1)})$ corresponds to a $\mathcal{N}(X^{(t)},1)$ density, depending on $X^{(t)}$ only.

② a stochastic sequence of binary random variables $\{X^{(t)}\}$, where $X^{(t)} = 1$ with probability p_t , and p_t is generated from a Beta $(3 + X^{(t-1)}, 3 - X^{(t-1)})$.

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Properties of a Markov chain

For the most part, the Markov chains encountered in Markov Chain Monte Carlo (MCMC) settings enjoy some fundamental properties.

- Irreducibility The kernel K allows for free moves all over the state-space: no matter the starting value $X^{(0)}$, the sequence $\{X^{(t)}\}$ has a positive probability of eventually reaching any region of the state-space.
- 2 Positive Recurrency The chain will return to any arbitrary nonnegible set an infinite number of times, with a finite expected return time.
- Aperiodicity The only length of time for which the chain repeats some cycle of values is the trivial case with cycle length equal to one.
- Stationarity There exists a probability distribution f such that if $X^{(t)} \sim f$, then $X^{(t+1)} \sim f$. Therefore, formally the kernel and the stationary distribution satisfy the equation:

$$\int_{\mathcal{X}} K(x,y) f(x) dx = f(y)$$

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Stationarity and limiting distribution

In Bayesian terms, our Markov chain is a bunch of draws $\{\theta^{(s)}\}$ of θ that are each slightly dependent on the previous one, and the posterior π is our target density f. The chain wanders around the parameter space, remembering only where it has been in the last period.

•———•

The fourth property, **stationarity**, is fundamental in MCMC setting. In case of recurrent chains, the stationary distribution is also a *limiting* distribution, in the sense that the limiting distribution of $\theta^{(s)}$ as $s \to \infty$ is π for almost any initial value $\theta^{(0)}$.

•

This fifth property is also called ergodicity, and it obviously has major consequences from a simulation point of view in that, if a given kernel K produces an ergodic Markov chain with stationary distribution π , generating a chain from this kernel K will eventually produce simulations from π .

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Monte Carlo Integration on the Markov Chain

Once we have a Markov chain that has converged to the stationary distribution, then the draws in our chain appear to be like draws from $\pi(\theta|y)$.

So it seems like we should be able to use Monte Carlo Integration methods to find our quantities of interest. One problem: our draws are not independent, and this assumption is required for Monte Carlo Integration to work. Remember the Strong Law of Large Numbers: if $\theta^{(1)}, \ldots, \theta^{(S)}$ are *iid* with mean $\mu = E(\theta^{(s)})$, then with probability 1:

$$\frac{1}{S} \sum_{s=1}^{S} \theta^{(s)} \to \mu \quad \text{a.s., as } S \to \infty.$$

Luckily, we have the Ergodic Theorem for correlated samples.

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The Ergodic theorem

The following theorem means suggests that the Strong Law of Large Numbers that lies at the basis of Monte Carlo methods can also be applied in MCMC settings.

Theorem (The Ergodic Theorem)

Given S values $\theta^{(1)}, \theta^{(2)}, \dots, \theta^{(S)}$ from a Markov chain that is aperiodic, irreducible, and positive recurrent (then the chain is called ergodic), and let $h: \Theta \to \mathbb{R}$ a real and integrable function such that $E(h(\theta)) < \infty$. Then with probability 1, as $S \to \infty$

$$\frac{1}{S} \sum_{s=1}^{S} h(\theta^{(s)}) \to \int_{\Theta} h(\theta) f(\theta) d\theta, \tag{2}$$

where the target distribution $f(\cdot)$ is the stationary distribution of the chain.

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Comments to the Ergodic theorem

- This is the Markov chain analogue to the SLLN, and it allows us to ignore the dependence between draws of the Markov chain when we calculate quantities of interest from the draws. The stationary distribution is also a limiting distribution.
- The asymptotic variance of a MCMC estimator is approximately:

$$S^{-1}\sigma^2(1+2\sum_{s}\rho_s),$$

where ρ_s is the s-th lag autocorrelation of the sequence (it behaves like a penalty).

 We will rely on MCMC algorithms—such as Metropolis-Hasting and Gibbs sampling—which are almost always theoretically convergent, meaning that the algorithm always converges to the stationary distribution f.

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How Does a Markov Chain Work - Discrete example

For discrete state space with k possible states, the transition kernel K is defined as a $k \times k$ matrix of transition probabilities:

$$P = \begin{bmatrix} Pr(A|A) & Pr(B|A) & Pr(C|A) & \dots & Pr(k|A) \\ Pr(A|B) & Pr(B|B) & & \dots & Pr(k|B) \\ \dots & & & & & \\ Pr(A|k) & Pr(B|k) & & \dots & Pr(k|k) \end{bmatrix}$$

where the first row expresses the probabilities of reaching any other state from state A in **one step**, and so on for the other rows. Thus, we may define $\Pr(\theta^{(s+1)} = A | \theta^{(s)} = B), \forall s$. Notice that the transition kernel does not depend on s. We say that the chain is homogeneous.

The **goal** is to generate $\theta^{(1)}, \ldots, \theta^{(S)}$ from the stationary distribution underlying the chain.

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How Does a Markov Chain Work - Discrete example

Suppose that k = 6 and that P is:

$$P = \begin{bmatrix} 0.5 & 0.5 & 0 & 0 & 0 & 0 \\ 0.25 & 0.5 & 0.25 & 0 & 0 & 0 \\ 0 & 0.25 & 0.5 & 0.25 & 0 & 0 \\ 0 & 0 & 0.25 & 0.5 & 0.25 & 0 \\ 0 & 0 & 0 & 0.25 & 0.5 & 0.25 \\ 0 & 0 & 0 & 0 & 0.5 & 0.5 \end{bmatrix}$$

where

$$\Pr(\theta^{(s+1)} = B | \theta^{(s)} = A) = 0.5$$

 $\Pr(\theta^{(s+1)} = C | \theta^{(s)} = B) = 0.25$

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How Does a Markov Chain Work - Discrete example

- (1) Define an initial vector of probabilities of length k, $\pi^{(0)}$.
- (2) At iteration 1, the distribution $\pi^{(1)}$ from which $\theta^{(1)}$ will be generated is given by:

$$\pi^{(1)} = \pi^{(0)}P$$

(3) At iteration 2, the distribution $\pi^{(2)}$ - from which $\theta^{(2)}$ will be generated - is given by:

$$\pi^{(2)} = \pi^{(1)}P = \pi^{(0)}P^2$$

- (4) ...
- (s) At iteration s, the distribution $\pi^{(s)}$ from which $\theta^{(s)}$ will be generated is given by:

$$\pi^{(s)} = \pi^{(s-1)}P = \pi^{(0)}P^s$$

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How Does a Markov Chain Work - Discrete example

We may find the **unique**, invariant distribution, i.e. a probability vector π such that

$$\pi = \pi P \tag{3}$$

In our example this vector is $\pi = (0.1, 0.2, 0.2, 0.2, 0.2, 0.1)$.

For all the MCMC algorithms we use in Bayesian statistics, the Markov chain will typically converge to π , regardless of our starting points.

So if we can devise a Markov chain whose stationary distribution π is our desired posterior distribution— $\pi(\theta|y)$ —then we can run this chain to get draws that can be considered as approximately drawn from $\pi(\theta|y)$, once the chain has converged.

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Thinning

Once we have a Markov chain that has converged to the stationary distribution, then the draws in our chain appear to be like draws from $\pi(\theta|y)$.

In order to break the dependence between draws in the Markov chain, some have suggested only keeping every d-th draw of the chain. This is known as thinning.

- **Pros**: Perhaps gets you a little closer to *iid* draws. Saves memory since you only store a fraction of the draws.
- Cons: Unnecessary with ergodic theorem. Shown to increase the variance of your Monte Carlo estimates.

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MCMC methods

MCMC is a class of methods in which we can simulate draws that are slightly dependent and are approximately from a (posterior) distribution.

We then take those draws and calculate quantities of interest for the (posterior) distribution.

In Bayesian statistics, there are generally two MCMC algorithms that we use:

- Metropolis-Hastings algorithm
- Gibbs sampling

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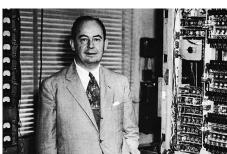
Metropolis-Hastings

History

- Monte Carlo: used by Enrico Fermi, 1930s, while studying neutron diffusion.
- MCMC The modern version was invented in the late 1940s by Stanislaw Ulam, while he was working on nuclear weapons projects at the Los Alamos National Laboratory. John Von Neumann programmed the ENIAC computer to carry out Monte Carlo calculations.







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Metropolis-Hastings algorithm

Suppose we have a posterior $\pi(\theta|y)$ that we want to sample from, but

- the posterior does not look like any distribution we know (no conjugacy...)
- the posterior consists of more than 2 parameters (grid approximations intractable)
- some (or all) of the full conditionals do not look like any distributions we know (thus, Gibbs sampling is unfeasible)

If all else fails, we can use the Metropolis-Hastings algorithm, which will always work, at least in theory.

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Basic Metropolis Hastings

- Choose a starting value $\theta^{(0)}$.
- ② At iteration s, given $\theta^{(s-1)}$, draw a candidate θ^* from a proposal (instrumental) distribution $g(\theta^*|\theta^{(s-1)})$.
- Compute the acceptance ratio:

$$R = \frac{\pi(\theta^*|y)g(\theta^{(s-1)}|\theta^*)}{\pi(\theta^{(s-1)}|y)g(\theta^*|\theta^{(s-1)})}.$$
 (4)

- **©** Compute the accept probability as $\rho = \min\{R, 1\}$.
- The value at iteration s is:

$$\theta^{(s)} = \begin{cases} \theta^* & \text{with probability } \rho \\ \theta^{(s-1)} & \text{wth probability } 1 - \rho \end{cases}$$

o Repeat steps 2-5 and get S samples $\theta^{(1)}, \ldots, \theta^{(S)}$.

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Step 1: choosing a starting value

- Under some easily satisfied regularity conditions on the proposal density $g(\theta^*|\theta^{(s-1)})$, the sequence $\theta^{(1)},\ldots,\theta^{(S)}$ will converge to a random variable (limiting distribution) that is distributed according to the posterior distribution $\pi(\theta|y)$.
- The important thing to remember is that $\theta^{(0)}$ must have positive probability, that is $\pi(\theta^{(0)}|y) > 0$.

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Step 2: draw θ^* from the proposal distribution

- The proposal $g(\theta^*|\theta^{(s-1)})$ determines where we move to in the next iteration of the Markov chain (analogous to the transition kernel).
- The support of g must contain the support of the posterior.
- Different M-H algorithms are constructed depending on the choice of proposal density:
 - Independent M-H: if the proposal density g is independent of the current value:

$$g(\theta^*|\theta^{(s-1)}) = g(\theta^*).$$

• Random Walk M-H: if the proposal density g is symmetric around zero, that is satisfying $g(\theta^*|\theta^{(s-1)}) \equiv h(\theta^*-\theta^{(s-1)})$. It yields that $g(\theta^{(s-1)}|\theta^*) \equiv h(\theta^{(s-1)}-\theta^*)$ and the acceptance ratio (4) has the simple form:

$$R = \frac{\pi(\theta^*|y)}{\pi(\theta^{(s-1)}|y)}.$$

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Step 2: draw θ^* from the proposal distribution

- ullet In the Independent M-H all our candidate draws $heta^*$ are drawn from the same distribution, regardless of where the previous draw was. This can be extremely efficient or extremely inefficient, depending on how close the proposal distribution is to the posterior. In general, chain will behave well only if the proposal distribution has heavier tails than the posterior.
- In the Random-Walk M-H the acceptance probability does not depend on g. This means that, for a given pair $(\theta^{(s-1)}, \theta^*)$, the probability of acceptance is the same whether $heta^*$ is generated from a Normal or a Cauchy distribution.

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Step 3: compute acceptance probability ρ

• The acceptance probability is:

$$\rho = \min \left\{ 1, \frac{\pi(\theta^*|y)g(\theta^{(s-1)}|\theta^*)}{\pi(\theta^{(s-1)}|y)g(\theta^*|\theta^{(s-1)})} \right\}.$$

In the case where proposal distribution is symmetric, we have that $g(\theta^*|\theta^{(s-1)}) = g(\theta^{(s-1)}|\theta^*)$, thus:

$$\rho = \min \left\{ 1, \frac{\pi(\theta^*|y)}{\pi(\theta^{(s-1)}|y)} \right\}.$$

- If our candidate draw has higher probability than our current draw, then our candidate is better ⇒ so we definitely accept it. Otherwise, our candidate is accepted according to the probability ratio (4).
- Since ρ is a ratio, we only need $\pi(\theta|y)$ up to a constant of proportionality, since p(y) cancels out in both the numerator and denominator.

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Step 3: compute acceptance probability ρ

- In cases where our proposal distribution is not symmetric, we need to weight our evaluations of the draws at the posterior densities by how likely we are to draw each draw.
- For example, if we are very likely to jump to some θ^* , then $g(\theta^*|\theta^{(s-1)})$ is likely to be high, so we should accept less of them than some other θ^* that we are less likely to jump to.

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Step 4: decide whether to accept θ^*

- Accept θ^* as your $\theta^{(s)}$ with probability ρ . If θ^* is not accepted, then $\theta^{(s)} = \theta^{(s-1)}$. Practically, how we do this?
 - For each θ^* , draw a value $U \sim \mathsf{Unif}(0,1)$.
 - ② If $U \le \rho$, accept θ^* ; otherwise, use $\hat{\theta}^{(s-1)} = \theta^{(s)}$. Candidate draws with higher density than the current draw are always accepted.
 - **1** Unlike in rejection sampling (A-R method), each iteration always produces a draw, either $\theta^{(s-1)}$ or θ^* .
- Now, we have to analyse the acceptance rate of our M-H algorithm. It
 is very important to monitor the acceptance rate, that is the fraction
 of candidate draws that are accepted, of our M-H algorithm.

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M-H acceptance rate

- If your acceptance rate is too high, the chain is probably not mixing well (not moving around the parameter space quickly enough).
- If your acceptance rate is too low, your algorithm is too inefficient (rejecting too many candidate draws).
- There is a trade-off: we would like large jumps (updates), so that the chain explores the state space, but large jumps usually have low acceptance probability as the posterior density can be highly peaked (and you jump off the mountain side)
- What is too high and too low depends on your specific algorithm, but generally:
 - random walk: somewhere between 0.25 and 0.50 is recommended
 - independent chain: something close to 1 is preferred

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A simple example: random-walk M-H for a Gamma(4.4, 1.7)

Gaussian proposal distribution with standard deviation 2.

```
Define a function for the entire M-H with fixed arguments
    # n.sims: number of simulations (samples)
    # start = starting value for theta_0
    # burnin = throw out a certain number of the first draws
    # cand.sd = sd of the normal proposal
    # shape, rate = gamma arguments
mh.gamma <-
  function(n.sims=10^5, start=1, burnin=0.3*n.sims, cand.sd=2,
           shape=1, rate=1) {
    # (1) initialization for theta 0 and definition of the draws
    theta.cur <- start
    draws <- c()
```

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Ex 1: random-walk M-H for a Gamma(4.4, 1.7)

R code continuation:

```
# (2) sampling from a normal with mean
       equal to the last value and sd = sd
theta.update <- function(theta.cur, shape, rate) {</pre>
  theta.can <- rnorm(1, mean = theta.cur, sd = cand.sd)
# (3) accept probability
  accept.prob <- dgamma(theta.can, shape = shape, rate = rate)/
    dgamma(theta.cur, shape = shape, rate = rate)
# (4) accept step
  if (runif(1) <= accept.prob)</pre>
    theta.can
  else theta.cur
}
```

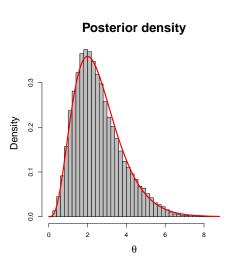
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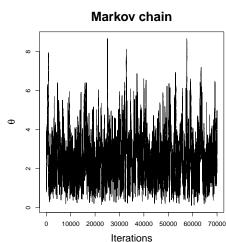
Ex 1: random-walk M-H for a Gamma(4.4, 1.7)

R code continuation:

```
# store the final draws
for (i in 1:n.sims) {
    draws[i] <- theta.cur <- theta.update(theta.cur,</pre>
                         shape = shape, rate = rate)}
# plots
samp<-draws[(burnin+1):n.sims]</pre>
par(mfrow=c(1,2))
hist(samp, nclass=50, prob=T,
      main="Posterior density",
      col="grey", xlab=expression(theta), cex.lab=2, cex.main=2)
curve(dgamma(x, shape=shape, rate=rate), add=T, lwd =3,
      col ="red")
plot(samp, type="1", ylab=expression(theta), xlab="Iterations",
  cex.lab=2, cex.main=2, main="Markov chain")
return(samp)}
```

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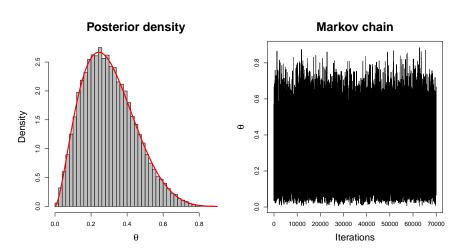


Figure: $g(\theta) = \text{Unif}(0,1)$. Acceptance rate = 0.503

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Ex 2: independent M-H for a Beta(2.7, 6.3)

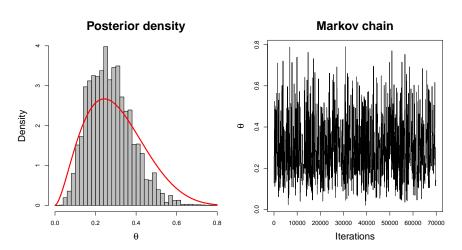


Figure: $g(\theta) = \text{Unif}(0,3)$. Acceptance rate = 0.12

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Suppose to have the following data coming from some shuttle flight measurements:

where we registered the number of failures Y for each of the n=23flights, at a given temperature (Fahrenheit) x.

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We suppose a simple binomial model for Y:

$$\Pr(Y_i = y) = {6 \choose y} \pi_i^y (1 - \pi_i)^{6-y},$$

where π_i is the failure probability for the *i*-th flight:

$$\pi_{i} = \frac{\exp\{\beta_{0} + \beta_{1}x_{i}\}}{1 + \exp\{\beta_{0} + \beta_{1}x_{i}\}}$$

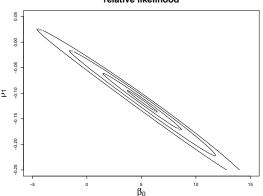
and x_i is the temperature value. The log-likelihood is then:

$$I(\beta_0, \beta_1) = \sum_{i=1}^n y_i (\beta_0 + \beta_1 x_i) - \sum_{i=1}^n 6 \log(1 + \exp{\{\beta_0 + \beta_1 x_i\}}).$$

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```
loglik <- function(beta) {
  sum(y * (beta[1] + beta[2] * x)) -
   sum(6 * log(1 + exp(beta[1] + beta[2]*x)))}</pre>
```





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We elicit a uniform prior distribution for β_0 and β_1 , $\pi(\beta_0, \beta_1) \propto 1$. The posterior is then proportional to:

$$\pi(\beta_0, \beta_1|y) \propto p(y|\beta_0, \beta_1)\pi(\beta_0, \beta_1) = \frac{\exp\{\sum_{i=1}^n y_i(\beta_0 + \beta_1 x_i)\}}{\prod_{i=1}^n [1 + \exp\{\beta_0 + \beta_1 x_i\}]}.$$

The posterior above is not known...We need MCMC simulation. So, we set up a random-walk Metropolis with the following proposal distributions at iteration s:

$$eta_0^* \sim \mathcal{N}(eta_0^{(s-1)}, s_1) \ eta_1^* \sim \mathcal{N}(eta_1^{(s-1)}, s_2)$$

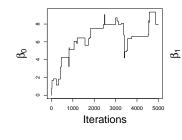
where s_1, s_2 are the instrumental variances.

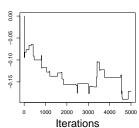
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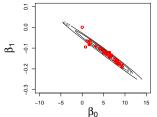
```
mh <- function(nsim, s1, s2, b.init) {
    mh.out <- matrix(ncol = 2, nrow = nsim)
    b <- b.init
    for (i in 1:nsim) {
        b.p <- c(rnorm(1, b[1], s1), rnorm(1,b[2], s2))
        if (runif(1) < exp(loglik(b.p) - loglik(b)))
        b <- b.p
        mh.out[i, ] <- b
        }
    mh.out}</pre>
```

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Scenario 1: $s_1 = s_2 = 1$. Poor mixing!

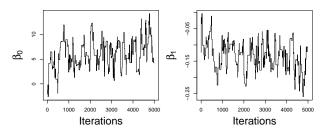


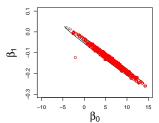




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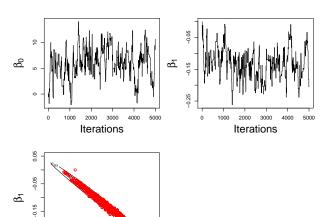
Scenario 2: $s_1=2,\ s_2=0.1.$ Better, still not adequate...





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Scenario 3: s_1, s_2 estimated from Scenario 2. Better, still not good...



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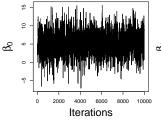
Consider now a correlated bivariate normal for the proposal distribution:

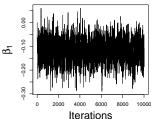
$$\begin{pmatrix} \beta_0^* \\ \beta_1^* \end{pmatrix} \sim \mathcal{N} \left(\begin{pmatrix} \beta_0^{(t-1)} \\ \beta_1^{(t-1)} \end{pmatrix}, \begin{pmatrix} \sigma_0^2 & \mathsf{Cov}(\beta_0, \beta_1) \\ \mathsf{Cov}(\beta_1, \beta_0) & \sigma_1^2 \end{pmatrix} \right).$$

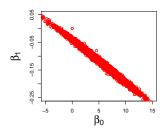
```
library(mvtnorm)
mhd <- function(nsim, V, b.init) {
   mh.out <- matrix(ncol = 2, nrow = nsim)
   b <- b.init
   for (i in 1:nsim) {
      b.p <- rmvnorm(n = 1, mean = b, sigma = V)
      if (runif(1) < exp(loglik(b.p) - loglik(b)))
       b <- b.p
      mh.out[i, ] <- b
    }
   mh.out}</pre>
```

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Scenario 4: cov.matrix V estimated from Scenario 3. Better!



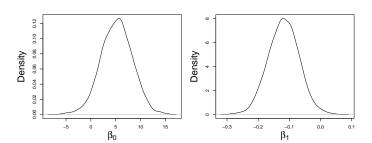




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- When there is a not negligible parameters' correlation, a suited proposal should capture this fact.
- We can use the last simulation to report posterior summaries for β_0 and β_1 .

```
apply(mh.out4,2, mean)
[1] 5.2003928 -0.1185773
```



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