

MCMC Package Example (Version 0.5-1)

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1 The Problem

This is an example of using the `mcmc` package in R. The problem comes from a take-home question on a (take-home) PhD qualifying exam (School of Statistics, University of Minnesota).

Simulated data for the problem are in the file `logit.txt`. There are five variables in the data set, the response `y` and four predictors, `x1`, `x2`, `x3`, and `x4`.

A frequentist analysis for the problem is done by the following R statements

```
> foo <- read.table("logit.txt", header = TRUE)
> out <- glm(y ~ x1 + x2 + x3 + x4, data = foo,
+   family = binomial())
> summary(out)
```

Call:

```
glm(formula = y ~ x1 + x2 + x3 + x4, family = binomial(), data = foo)
```

Deviance Residuals:

Min	1Q	Median	3Q	Max
-1.7461	-0.6907	0.1540	0.7041	2.1943

Coefficients:

	Estimate	Std. Error	z value	Pr(> z)
(Intercept)	0.6328	0.3007	2.104	0.03536 *
x1	0.7390	0.3616	2.043	0.04100 *
x2	1.1137	0.3627	3.071	0.00213 **
x3	0.4781	0.3538	1.351	0.17663
x4	0.6944	0.3989	1.741	0.08172 .

Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

(Dispersion parameter for binomial family taken to be 1)

Null deviance:	137.628	on 99	degrees of freedom
Residual deviance:	87.668	on 95	degrees of freedom

AIC: 97.668

Number of Fisher Scoring iterations: 6

But this problem isn't about that frequentist analysis, we want a Bayesian analysis. For our Bayesian analysis we assume the same data model as the frequentist, and we assume the prior distribution of the five parameters (the regression coefficients) makes them independent and identically normally distributed with mean 0 and standard deviation 2.

The log unnormalized posterior (log likelihood plus log prior) density for this model is calculated by the following R function (given the preceding data definitions)

```
> x <- foo
> x$y <- NULL
> x <- as.matrix(x)
> x <- cbind(1, x)
> dimnames(x) <- NULL
> y <- foo$y
> lupost <- function(beta, x, y) {
+   eta <- x %*% beta
+   p <- 1/(1 + exp(-eta))
+   logl <- sum(log(p[y == 1])) + sum(log(1 -
+     p[y == 0]))
+   return(logl + sum(dnorm(beta, 0, 2, log = TRUE)))
+ }
```

2 Beginning MCMC

With those definitions in place, the following code runs the Metropolis algorithm to simulate the posterior.

```
> library(mcmc)
> set.seed(42)
> beta.init <- as.numeric(coefficients(out))
> out <- metrop(lupost, beta.init, 1000, x = x,
+   y = y)
> names(out)

[1] "accept"      "batch"      "initial"
[4] "final"      "initial.seed" "final.seed"
[7] "time"       "lud"       "nbatch"
[10] "blen"      "nspac"     "scale"

> out$accept

[1] 0.008
```

The arguments to the `metrop` function here (there are more we don't use here) are

- an R function (here `lupost` that evaluates the log unnormalized density of the desired stationary distribution (here a posterior distribution) of the Markov chain. Note that (although this example does not exhibit the phenomenon) that the unnormalized density may be zero, in which case the log unnormalized density is `-Inf`.
- an initial state (here `beta.init`) of the Markov chain.
- a number of batches (here `1e3`) for the Markov chain. This combines with batch length and spacing (both 1 by default) to determine the number of iterations done.
- additional arguments (here `x` and `y`) supplied to provided functions (here `lupost`).
- there is no “burn-in” argument, although burn-in is easily accomplished, if desired (more on this below).

The output is in the component `out$batch` returned by the `metrop` function. We'll look at it presently, but first we need to adjust the proposal to get a higher acceptance rate (`out$accept`). It is generally accepted (Gelman, Roberts, and Gilks, 1996) that an acceptance rate of about 20% is right, although this recommendation is based on the asymptotic analysis of a toy problem (simulating a multivariate normal distribution) for which one would never use MCMC and is very unrepresentative of difficult MCMC applications.

Geyer and Thompson (1995) came to a similar conclusion, that a 20% acceptance rate is about right, in a very different situation. But they also warned that a 20% acceptance rate could be very wrong and produced an example where a 20% acceptance rate was impossible and attempting to reduce the acceptance rate below 70% would keep the sampler from ever visiting part of the state space. So the 20% magic number must be considered like other rules of thumb we teach in intro courses (like $n > 30$ means normal approximation is valid). We know these rules of thumb can fail. There are examples in the literature where they do fail. We keep repeating them because we want something simple to tell beginners, and they are all right for some problems.

Be that as it may, we try for 20%.

```
> out <- metrop(out, scale = 0.1, x = x, y = y)
> out$accept
```

```
[1] 0.739
```

```
> out <- metrop(out, scale = 0.3, x = x, y = y)
> out$accept
```

```
[1] 0.371
```

```

> out <- metrop(out, scale = 0.5, x = x, y = y)
> out$accept

[1] 0.148

> out <- metrop(out, scale = 0.4, x = x, y = y)
> out$accept

[1] 0.209

```

Here the first argument to each instance of the `metrop` function is the output of a previous invocation. The Markov chain continues where the previous run stopped doing just what it would have done if it had kept going the initial state and random seed being the final state and random seed of the previous invocation. Everything stays the same except for the arguments (here `scale` that are supplied).

- The argument `scale` controls the size of the Metropolis “normal random walk” proposal. The default is `scale = 1`. Big steps give lower acceptance rates. Small steps give higher. We want something about 20%. It is also possible to make `scale` a vector or a matrix. See `help(metrop)`.

Because each run starts where the last one stopped (when the first argument to `metrop` is the output of the previous invocation), each run serves as “burn-in” for its successor (assuming that any part of that run was worth anything at all).

3 Diagnostics

O. K. That does it for the acceptance rate. So let’s do a longer run and look at the results.

```

> out <- metrop(out, nbatch = 10000, x = x, y = y)
> out$accept

[1] 0.2345

> out$time

[1] 1.15 0.00 1.17 0.00 0.00

```

Figure 1 (page 5) shows the time series plot made by the R statement

```
> plot(ts(out$batch))
```

Another way to look at the output is an autocorrelation plot. Figure 2 (page 6) shows the time series plot made by the R statement

```
> acf(out$batch)
```

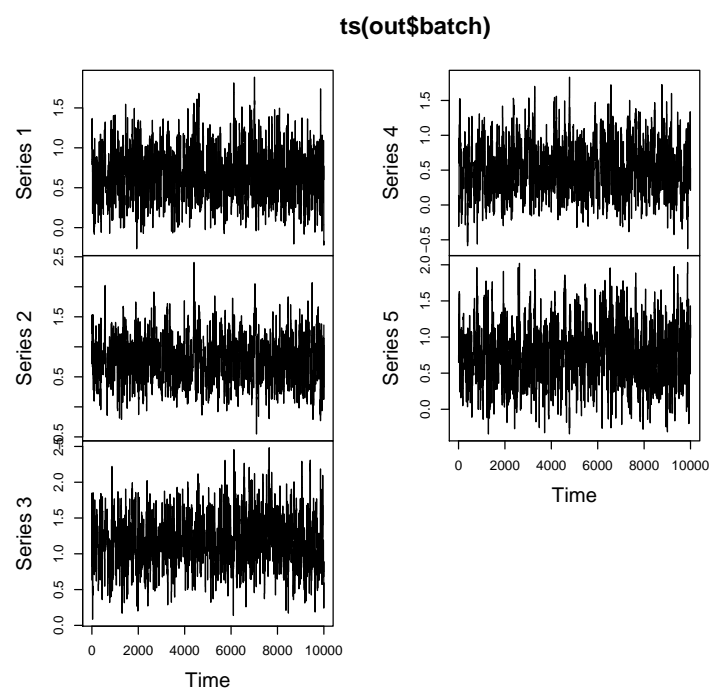


Figure 1: Time series plot of MCMC output.

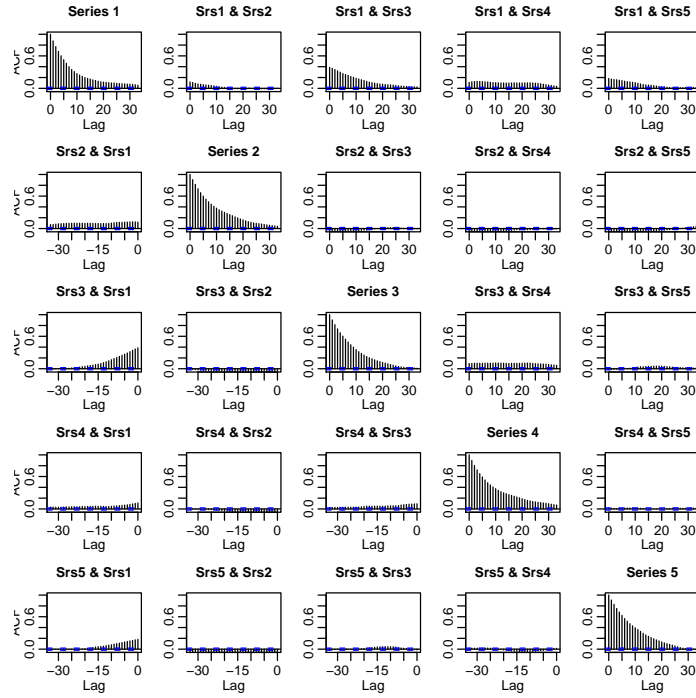


Figure 2: Autocorrelation plot of MCMC output.

As with any multiplot plot, these are a bit hard to read. Readers are invited to make the separate plots to get a better picture. As with all “diagnostic” plots in MCMC, these don’t “diagnose” subtle problems. As

<http://www.stat.umn.edu/~charlie/mcmc/diag.html>

says

The purpose of regression diagnostics is to find obvious, gross, embarrassing problems that jump out of simple plots.

The time series plots will show *obvious* nonstationarity. They will not show *nonobvious* nonstationarity. They provide no guarantee whatsoever that your Markov chain is sampling anything remotely resembling the correct stationary distribution (with log unnormalized density `lupost`). In this very easy problem, we do not expect any convergence difficulties and so believe what the diagnostics seem to show, but one is a fool to trust such diagnostics in difficult problems.

The autocorrelation plots seem to show that the autocorrelations are negligible after about lag 25. This diagnostic inference is reliable if the sampler is actually working (has nearly reached equilibrium) and worthless otherwise. Thus batches of length 25 should be sufficient, but let’s use length 100 to be safe.

4 Monte Carlo Estimates and Standard Errors

```
> out <- metrop(out, nbatch = 100, blen = 100, outfun = function(z,
+ ...) c(z, z^2), x = x, y = y)
> out$accept

[1] 0.2332

> out$time

[1] 1.16 0.00 1.17 0.00 0.00
```

We have added an argument `outfun` that gives the “functional” of the state we want to average. For this problem we are interested in both posterior mean and variance. Mean is easy, just average the variables in question. But variance is a little tricky. We need to use the identity

$$\text{var}(X) = E(X^2) - E(X)^2$$

to write variance as a function of two things that can be estimated by simple averages. Hence we want to average the state itself and the squares of each component. Hence our `outfun` returns `c(z, z^2)` for an argument (the state vector) `z`.

The `...` argument to `outfun` is required, since the function is also passed the other arguments (here `x` and `y`) to `metrop`.

4.1 Simple Means

The grand means (means of batch means) are

```
> apply(out$batch, 2, mean)

[1] 0.6531950 0.7920342 1.1701075 0.5077331 0.7488265
[6] 0.5145751 0.7560775 1.4973807 0.3913837 0.7244162
```

The first 5 numbers are the Monte Carlo estimates of the posterior means. The second 5 numbers are the Monte Carlo estimates of the posterior absolute second moments. We get the posterior variances by

```
> foo <- apply(out$batch, 2, mean)
> mu <- foo[1:5]
> sigmasq <- foo[6:10] - mu^2
> mu

[1] 0.6531950 0.7920342 1.1701075 0.5077331 0.7488265

> sigmasq

[1] 0.08791134 0.12875924 0.12822924 0.13359081 0.16367507
```

Monte Carlo standard errors (MCSE) are calculated from the batch means. This is simplest for the means.

```
> mu.mcse <- apply(out$batch[, 1:5], 2, sd)/sqrt(out$nbatch)
> mu.mcse

[1] 0.01224260 0.01417916 0.01793129 0.01468594 0.01582040
```

The extra factor `sqrt(out$nbatch)` arises because the batch means have variance σ^2/b where b is the batch length, which is `out$blen`, whereas the overall means `mu` have variance σ^2/n where n is the total number of iterations, which is `out$blen * out$nbatch`.

4.2 Functions of Means

To get the MCSE for the posterior variances we apply the delta method. Let u_i denote the sequence of batch means of the first kind for one parameter and \bar{u} the grand mean (the estimate of the posterior mean of that parameter), let v_i denote the sequence of batch means of the second kind for the same parameter and \bar{v} the grand mean (the estimate of the posterior second absolute moment of that parameter), and let $\mu = E(\bar{u})$ and $\nu = E(\bar{v})$. Then the delta method linearizes the nonlinear function

$$g(\mu, \nu) = \nu - \mu^2$$

as

$$\Delta g(\mu, \nu) = \Delta \nu - 2\mu \Delta \mu$$

saying that

$$g(\bar{u}, \bar{v}) - g(\mu, \nu)$$

has the same asymptotic normal distribution as

$$(\bar{v} - \nu) - 2\mu(\bar{u} - \mu)$$

which, of course, has variance `1 / nbatch` times that of

$$(v_i - \nu) - 2\mu(u_i - \mu)$$

and this variance is estimated by

$$\frac{1}{n_{\text{batch}}} \sum_{i=1}^{n_{\text{batch}}} [(v_i - \bar{v}) - 2\bar{u}(u_i - \bar{u})]^2$$

So

```
> u <- out$batch[, 1:5]
> v <- out$batch[, 6:10]
> ubar <- apply(u, 2, mean)
> vbar <- apply(v, 2, mean)
> deltau <- sweep(u, 2, ubar)
> deltav <- sweep(v, 2, vbar)
> foo <- sweep(deltav, 2, ubar, "*")
> sigmasq.mcse <- sqrt(apply((deltav - 2 * foo)^2,
+   2, mean)/out$nbatch)
> sigmasq.mcse

[1] 0.004241637 0.007292224 0.007271390 0.007374833
[5] 0.008175832
```

does the MCSE for the posterior variance.

Let's just check that this complicated `sweep` and `apply` stuff does do the right thing.

```
> sqrt(mean(((v[, 2] - vbar[2]) - 2 * ubar[2] *
+   (u[, 2] - ubar[2]))^2)/out$nbatch)

[1] 0.007292224
```

Comment Through version 0.5 of this vignette it contained an incorrect procedure for calculating this MCSE, justified by a handwave. Essentially, it said to use the standard deviation of the batch means called `v` here, which appears to be very conservative.

4.3 Functions of Functions of Means

If we are also interested in the posterior standard deviation (a natural question, although not asked on the exam problem), the delta method gives its standard error in terms of that for the variance

```
> sigma <- sqrt(sigmasq)
> sigma.mcse <- sigmasq.mcse/(2 * sigma)
> sigma

[1] 0.2964985 0.3588304 0.3580911 0.3655008 0.4045678

> sigma.mcse

[1] 0.007152882 0.010161102 0.010152989 0.010088669
[5] 0.010104403
```

5 A Final Run

So that's it. The only thing left to do is a little more precision (the exam problem directed “use a long enough run of your Markov chain sampler so that the MCSE are less than 0.01”)

```
> out <- metrop(out, nbatch = 500, blen = 400, x = x,
+             y = y)
> out$accept

[1] 0.235155

> out$time

[1] 23.40 0.02 24.40 0.00 0.00

> foo <- apply(out$batch, 2, mean)
> mu <- foo[1:5]
> sigmasq <- foo[6:10] - mu^2
> mu

[1] 0.6624650 0.7941013 1.1712710 0.5066326 0.7261414

> sigmasq

[1] 0.09189246 0.13323054 0.13230811 0.12871293 0.15978638

> mu.mcse <- apply(out$batch[, 1:5], 2, sd)/sqrt(out$nbatch)
> mu.mcse

[1] 0.002960128 0.003647420 0.003787855 0.003632080
[5] 0.004273624
```

```

> u <- out$batch[, 1:5]
> v <- out$batch[, 6:10]
> ubar <- apply(u, 2, mean)
> vbar <- apply(v, 2, mean)
> deltau <- sweep(u, 2, ubar)
> deltav <- sweep(v, 2, vbar)
> foo <- sweep(deltau, 2, ubar, "*")
> sigmasq.mcse <- sqrt(apply((deltav - 2 * foo)^2,
+ 2, mean)/out$nbatch)
> sigmasq.mcse

[1] 0.001044801 0.001725900 0.001518322 0.001553468
[5] 0.002010717

> sigma <- sqrt(sigmasq)
> sigma.mcse <- sigmasq.mcse/(2 * sigma)
> sigma

[1] 0.3031377 0.3650076 0.3637418 0.3587658 0.3997329

> sigma.mcse

[1] 0.001723311 0.002364198 0.002087087 0.002165017
[5] 0.002515076

```

and some nicer output, which is presented in three tables constructed from the R variables defined above using the R `xtable` command in the `xtable` library.

First the posterior means, then the posterior variances (table on page 11),

Table 1: Posterior Means

	constant	x_1	x_2	x_3	x_4
estimate	0.6625	0.7941	1.1713	0.5066	0.7261
MCSE	0.0030	0.0036	0.0038	0.0036	0.0043

and finally the posterior standard deviations (table on page 12).

Table 2: Posterior Variances

	constant	x_1	x_2	x_3	x_4
estimate	0.0919	0.1332	0.1323	0.1287	0.1598
MCSE	0.0010	0.0017	0.0015	0.0016	0.0020

Note for the record that the all the results presented in the tables are from “one long run” where long here took only 23.4 seconds (on whatever computer it was run on).

Table 3: Posterior Standard Deviations

	constant	x_1	x_2	x_3	x_4
estimate	0.3031	0.3650	0.3637	0.3588	0.3997
MCSE	0.0017	0.0024	0.0021	0.0022	0.0025

References

- Gelman, A., G. O. Roberts, and W. R. Gilks (1996). Efficient Metropolis jumping rules. In *Bayesian Statistics, 5 (Alicante, 1994)*, pp. 599–607. Oxford University Press.
- Geyer, C. J. and E. A. Thompson (1995). Annealing Markov chain Monte Carlo with applications to ancestral inference. *Journal of the American Statistical Association*, 90, 909–920.