An Introduction to Estimating Monte Carlo Standard Errors with R Package `mcmcse`

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1 Introduction

The R package mcmcse provides estimates of Monte Carlo standard errors for Markov chain Monte Carlo (MCMC) algorithms. This package is useful when estimating means and quantiles of functions of the MCMC output. In addition to MCMC output, the package can be used for time series and other correlated processes.
The package is predominantly useful after MCMC output has been obtained by the user. In addition to estimating the Monte Carlo standard errors, the package also provides basic graphical diagnostics and calculation of effective sample size. Various features in the package can be implemented using both multivariate and univariate methods.

2 An MCMC Example

To illustrate the use of our package, we present the following simple multivariate AR(1) process. The process is defined for $t = 1, 2, 3, \ldots$ is defined as,

$$y_t = w + Ay_{t-1} + \epsilon_t,$$

where w is a constant vector in $\mathbb{R}^p$, $y_t \in \mathbb{R}^p$, A is a $p \times p$ matrix and $\epsilon_t \sim N_p(0, C)$. In our example, we let A and C be diagonal matrices. The invariant distrbution for this process is $F = N_p(0, V)$ where V is a function of A and C.
The function mAr.sim in package mAr draws samples from the above model. We let $p = 3$.

```
library(mAr)

## Loading required package:  MASS

p <- 3
A <- diag(c(.1, .5, .8))
C <- diag(rep(2, 3))

set.seed(100)
chain <- mAr.sim(w = rep(2,p), A = A, C = C, N = 10000)
```

For using the mcmcse package the rows of the MCMC output should store each iteration of the algorithm. Thus the output should have n rows and p columns. We will denote each row i of the out put as $(y_i^{(1)}, y_i^{(2)}, y_i^{(3)})$.

This vignette will discuss estimating two sets of features of interest of F.

- the expectation of y, $E_F y$
- the expectation of sum of the second moments of all components of y, $E_F(y^{(1)2} + y^{(2)2} + y^{(3)2})$.

Suppose first we are interested in estimating $\mu = E_F y$. Then the estimator for that is just the sample mean

$$\mu_n = \frac{1}{n} \sum_{t=1}^{n} y_t.$$

μ_n is obtained using the usual `colMeans` function.

```
colMeans(chain)

##        X1       X2       X3
## 2.213455 3.989894 9.990273
```

Due to a central limit theorem argument,

$$\sqrt{n}(\mu_n - \mu) \xrightarrow{d} N_p(0, \Sigma). \tag{1}$$

Alternatively, we could also be interested in estimating say the sum of the second moments of each component of y. In this case, we define the function $g : \mathbb{R}^3 \to \mathbb{R}$ as $g((x_1, x_2, x_3)) = x_1^2 + x_2^2 + x_3^2$. This is defined in `R` by creating a function that takes a vector argument.

```
g <- function(x)
{
        return(sum(x^2))
}
```

The Monte Carlo estimate for g is

$$\mu_{g,n} = \frac{1}{n} \sum_{t=1}^{n} g(y_t),$$

and a CLT of the following form may be available

$$\sqrt{n}(\mu_{g,n} - \mu) \xrightarrow{d} N_p(0, \Sigma_g). \tag{2}$$

Finding the estimate and the Monte Carlo standard errors for $E_F g$ are explained in the following section.

3 Estimating Monte Carlo Standard Error

Using the `mcmcse` package we can estimate Σ in (1) with the `mcse.multi` function.

```
library(mcmcse)

## mcmcse:  Monte Carlo Standard Errors for MCMC
## Version 1.1-2 created on 17-08-2015.
## copyright (c) 2012, James M. Flegal, University of California,Riverside
##                     John Hughes, University of Minnesota
##                     Dootika Vats, University of Minnesota
##  For citation information, type citation("mcmcse").
##  Type help("mcmcse-package") to get started.

mcerror_bm <- mcse.multi(x = chain, method =  "bm",
        size = "sqroot", g = NULL, level = .95, large = FALSE)
mcerror_bart <- mcse.multi(x = chain, method =  "bartlett",
        size = "cuberoot", g = NULL, level = .95, large = FALSE)
mcerror_tuk <- mcse.multi(x = chain, method =  "tukey",
        size = "sqroot", g = NULL, level = .95, large = FALSE)
```

- `x` takes the $n \times p$ MCMC data. `x` can take only numeric entries in the form of a matrix or data frame. The rows of `x` are the iterations of the MCMC.

- `method = ‘‘bm’’, ‘‘bartlett’’, ‘‘tukey’’` calculates the estimate using the batch means method and spectral variance methods with the modified-Bartlett and Tukey-Hanning windows.

- `size` is the batch size for the `bm` method and the truncation point for `tukey` and `bartlett` methods. `size = ‘‘sqroot’’` sets the size as $\lfloor \sqrt{n} \rfloor$ and `size = ‘‘cuberoot’’` sets it at $\lfloor n^{1/3} \rfloor$. An integer value of `size` less than n is also valid.

- `g` is a function that is applied to each row of `x` and represents the features of interest of the process. Since here we are interested in only means, `g` is `NULL`. `g` will be explained in later examples.

- `level` is the confidence level of the resulting confidence region. This is required to calculate the volume of the confidence region.

- `large` is a logical argument. If `large` is `TRUE` the volume of the confidence region is the large sample volume obtained using χ^2 critical values. By default, volume is calculated using F distribution critical values.

`mcse.multi` returns a list with multiple components. `cov` stores the estimate of Σ obtained using the method chosen, `vol` returns the volume to the pth root of the resulting confidence region, `est` stores the estimate of g applied on the Markov chain and `nsim`, `critical` and `size` are useful to remember the methods used to calculate Σ.

```
mcerror_bm$cov

##             [,1]       [,2]       [,3]
## [1,]  2.1818978 -0.2932679  0.8416831
## [2,] -0.2932679  7.1329697  1.9953946
## [3,]  0.8416831  1.9953946 44.2180584

mcerror_bart$cov

##            [,1]       [,2]       [,3]
## [1,] 2.4769750  0.1504705  0.3108498
## [2,] 0.1504705  7.5311309 -0.2104305
## [3,] 0.3108498 -0.2104305 36.2779449

mcerror_tuk$cov

##            [,1]      [,2]      [,3]
## [1,] 2.5605087 0.1785598  1.291766
## [2,] 0.1785598 7.1818559  1.107386
## [3,] 1.2917665 1.1073863 46.506845

rbind(mcerror_bm$est, mcerror_bart$est, mcerror_tuk$est)

##             X1       X2       X3
## [1,] 2.213455 3.989894 9.990273
## [2,] 2.213455 3.989894 9.990273
## [3,] 2.213455 3.989894 9.990273

c(mcerror_bm$vol, mcerror_bart$vol, mcerror_tuk$vol)

## [1] 0.1370514 0.1335043 0.1384341
```

Note: The estimates are not affected by the choice of the method.

Note: The batch means estimators are significantly faster to calculate than the spectral variance estimators. The user is advised to use the default `method = ‘‘bm’’` for large input matrices.

Note: `cov` returns an estimate of Σ and not Σ/n.

If the diagonals of Σ are σ_{ii}^2, the function `mcse` and `mcse.mat` returns $\sigma_{ii}/\sqrt{n}$. `mcse` does it for one component and `mcse.mat` does it for all diagonals.

```
mcse(x = chain[,1], method = "bm", g = NULL)

## $est
## [1] 2.213455
##
## $se
## [1] 0.01477125

mcse.mat(x = chain, method = "bm", g = NULL)

##         est          se
## X1 2.213455 0.01477125
## X2 3.989894 0.02670762
## X3 9.990273 0.06649666
```

In order to estimate $\mu_{n,g}$ and Σ_g as in (2), we use the `R` function `g` we had defined before. Recall that `g` should be a funcation that takes vector inputs.

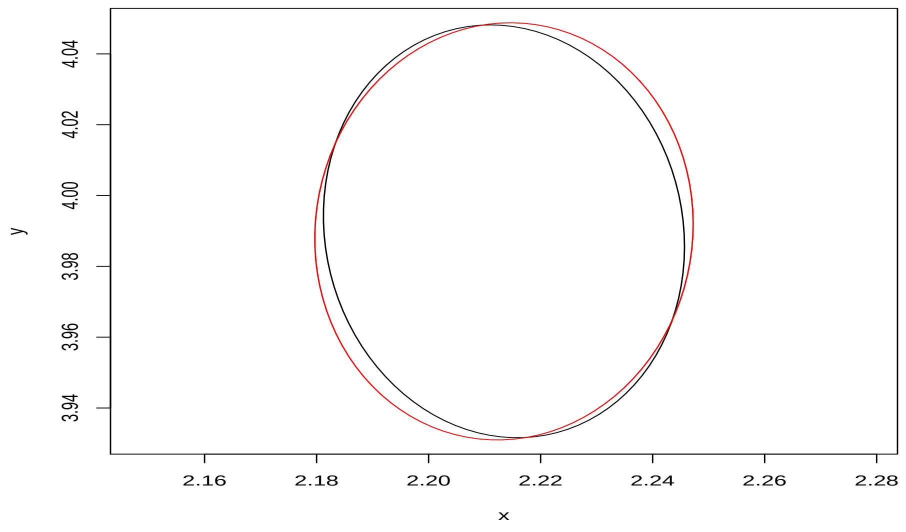
```
g

## function(x)
## {
##  return(sum(x^2))
## }

mcerror_g_bm <- mcse.multi(x = chain, g = g)

mcerror_g_bm$cov

##          [,1]
## [1,] 18247.05
```

```
mcerror_g_bm$est

## [1] 130.4437
```

4 Confidence Regions

Using the function `confRegion` in the package, the user can create joint confidence regions for two parameters. The input for this function is the output list from the `mcse.multi` function. The function uses the attributes `critical`, `est` and `nsim` from the `mcse.multi` output list.

```
plot(confRegion(mcerror_bm, which = c(1,2), level = .90), type = 'l', asp = 1)
lines(confRegion(mcerror_bart, which = c(1,2), level = .90), col = "red")
```



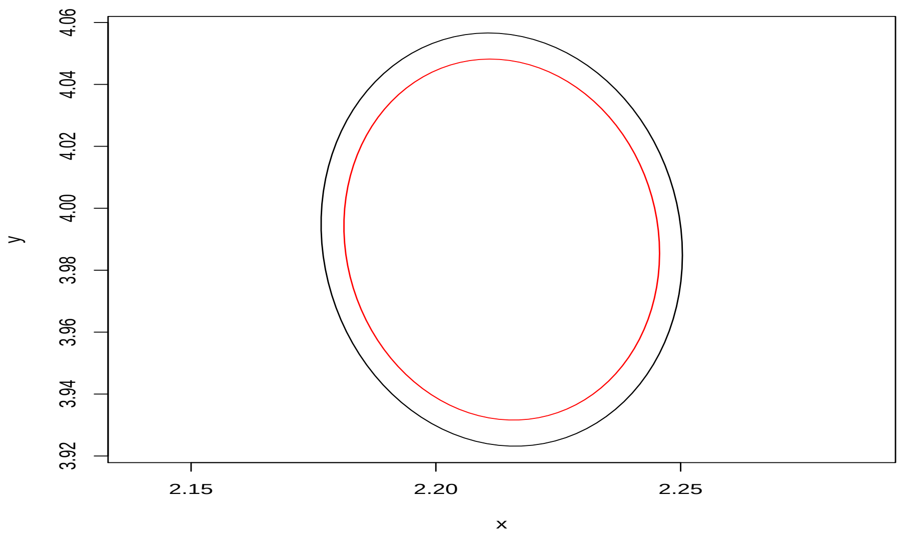
- `which` should be a vector of size 2 that indicates the two components for which the confidence ellipse is to be constructed.
- `level` is the confidence level of the confidence region. The default is .95

NOTE: The argument `confRegion` calls on the function `ellipse` in package `ellipse` to draw the ellipse.

NOTE: Since the confidence region is created for two parameters only, the size of the ellipse is determined by setting $p = 2$ irrespective of the original dimension of the problem.

To determine the effect of the confidence level, we draw two regions with difference confidence levels.

```
plot(confRegion(mcerror_bm, which = c(1,2), level = .95), type = 'l', asp = 1)
lines(confRegion(mcerror_bm, which = c(1,2), level = .90), col = "red")
```



5 Effective Sample Size

`multiESS` and `ess` are two functions that calculate the effective sample size of a correlated sample. `ess` calculations are based on Gong and Flegal (2015) and is component-wise, and `multiESS` utilizes the multivariate nature of the problem.

```
ess(chain)

##       X1       X2       X3
## 9381.155 3670.521 1165.908
```

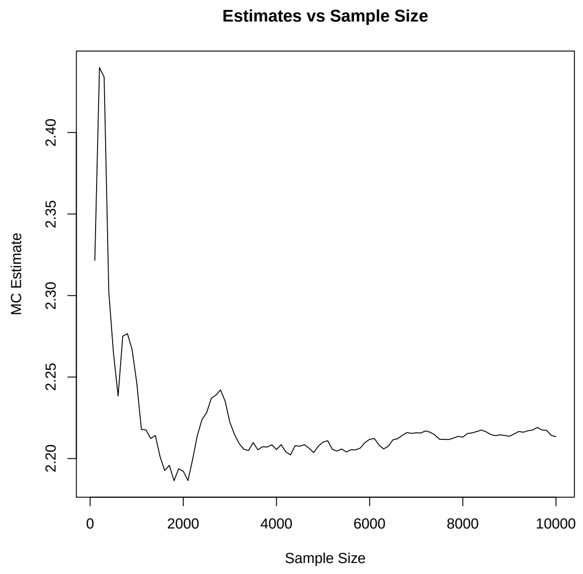
Since `ess` produces a different estimate for each component, conservative practice dictates choosing the smallest of the values. `multiESS` returns one estimate of the effective sample size based on the whole sample. The function calls `mcse.multi` function to obtain a batch means estimate of Σ. The user can provide another estimate of Σ using the `covmat` argument.

```
multiESS(chain)

## [1] 3455.318

multiESS(chain, covmat = mcerror_bart$cov)

## [1] 3446.062
```

6 Graphical Diagnostics

The function `estvssamp` plots the Monte Carlo estimates versus the sample size for a component of the MCMC output. This plot indicates whether the Monte Carlo estimate has stabilized.

```
estvssamp(chain[,1])
```

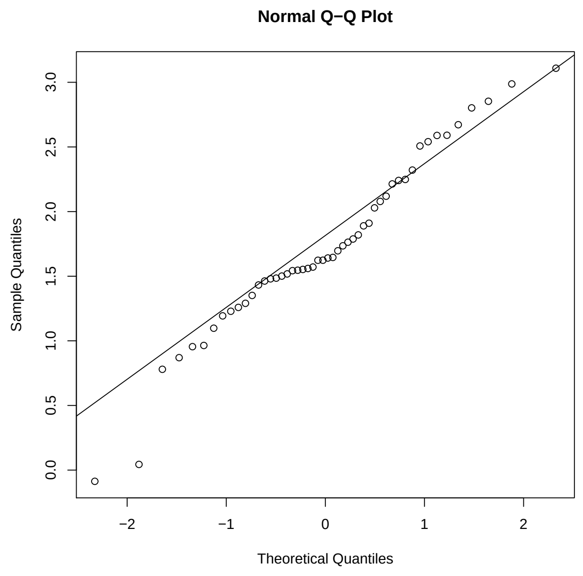


Additionally, if p is not too small, due to the central limit theorem in (1) and an estimate of Σ using the `mcse.multi` function, a QQ plot of the standardized estimates gives an idea of whether asymptopia has been achieved. We generate a new Markov chain with $p = 50$.

```
p <- 50
A <- diag(seq(.1, .9, length = p))
C <- diag(rep(2, p))

set.seed(100)
chain <- mAr.sim(w = rep(2,p), A = A, C = C, N = 10000)
```

For this new Markov chain, we find an estimate of Σ to use for the `qqTest` function.

```
mcerror_bm <- mcse.multi(chain, method = "bm")
qqTest(x = chain, covmat = mcerror_bm$cov)
```



Thus, we see here that the chain has not quite reached asymptopia.

References

Gong, L. and Flegal, J. M. (2015). A practical sequential stopping rule for high-dimensional markov chain monte carlo. *Journal of Computational and Graphical Statistics*, (just-accepted):00–00.