evolMC demo

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evolMC is a framework for doing Monte-Carlo simulations. The package, as of this writing, is not particularly optimized for speed, but to allow for the user to easily construct arbitrary MCMC schemes.

1.1 Univariate and multivariate sampling

We wish to use a metropolis sampler to draw from a distribution with density

$$f(x) \propto \frac{\sin(x)}{x} \cdot 1_{(0,\pi)}(x).$$

We can use a uniform distribution on $(-1, 1)$ to propose distances to jump from the current location.

Since the proposal distribution is symmetric, this is enough information to implement a Metropolis updater. We must implement a log-density function[1] that defines the distribution. We must also implement a proposal generation function.

```
ln.d <- function(x) log(sin(x)/x * (0 < x) * (x < pi))
propose <- function(x) x + runif(length(x), -1, 1)
```

The `metropolis` function accepts the functions that we have defined, and returns a new function. The returned function is an implementation of the Metropolis updating scheme you have defined.[2]

```
updater <- metropolis(ln.d, propose)
```

A Markov chain is formed by iteratively calling the updating function starting with some initial value. The `iterate` function forms a *chain object*, which is simply a list of states that the chain realized. If the state object is of a few particularly simple (but widely applicable) forms then there are convenient methods defined for several common R functions.

```
chain <- iterate(n = 10000, fn = updater, init = 1)
summary(chain, discard = 57)

## Discarding first 57 states.
##     mean       se    2.5%    97.5%
## 1.07001 0.73139 0.03456 2.63735
```

There is a method for the summary function that reports summary statistics for the chain. A method for the hist function will create a histogram from the chain object. By default, these methods discard the first 10% of values from the chain as a burn-in, but this may be altered if desired by the user.

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[1] Actually, this function need only be known up to the normalizing constant.

[2] If your proposal generator is not symmetric, then you must also supply a log-density for the proposal mechanism, and in this case the function returned will implement Metropolis-Hastings.

```
hist(chain, breaks = "fd")

## Discarding first 1000 states.
```

Histogram of m
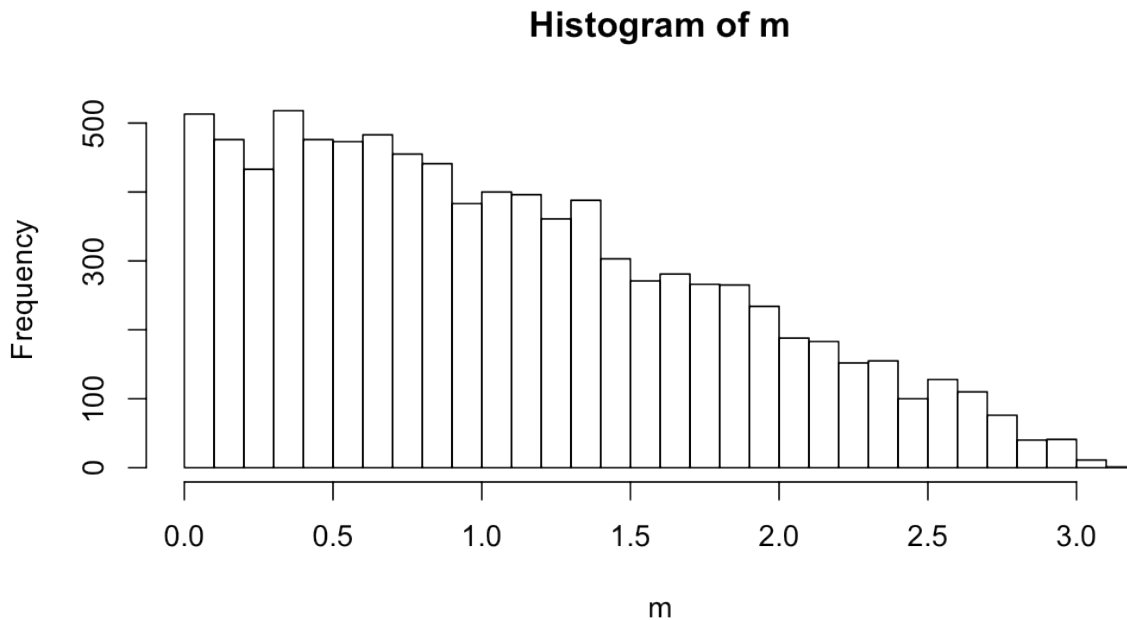
Of course, multivariate distributions may also be sampled. We need only define an appropriate multivariate log-density function. A quick review of the `propose` function we defined for the univariate sampler confirms that it will also work in the case when it is passed a vector. (Due to the `length(x)` rather than 1.) We pass these functions to `metropolis` and obtain our updating function, which is used with `iterate` to form the Markov chain.

```
mvtarget <- function(x) log(prod(sin(prod(x))/x) * all(x > 0, x < pi, prod(x) <
    pi))
mvupdate <- metropolis(mvtarget, propose)
chain2 <- iterate(10000, mvupdate, cbind(x = 1, y = 1))
summary(chain2)

## Discarding first 1000 states.
##             x      y
## mean   1.2738 1.2330
## se     0.8105 0.7910
## 2.5%   0.1703 0.1816
## 97.5% 3.0076 2.9277

plot(chain2)
```
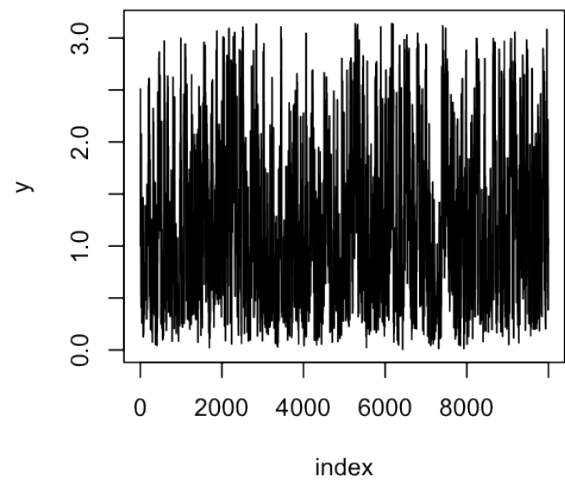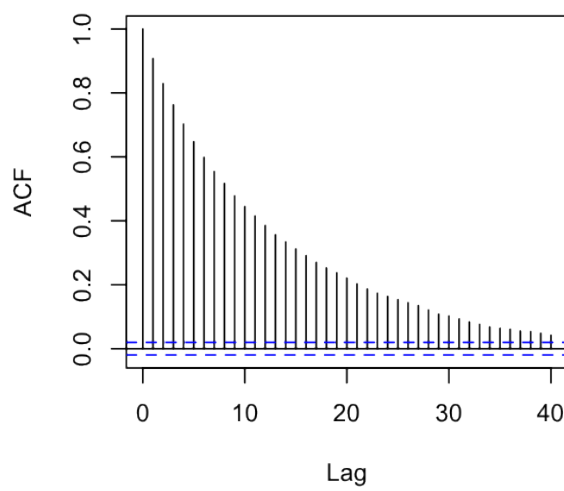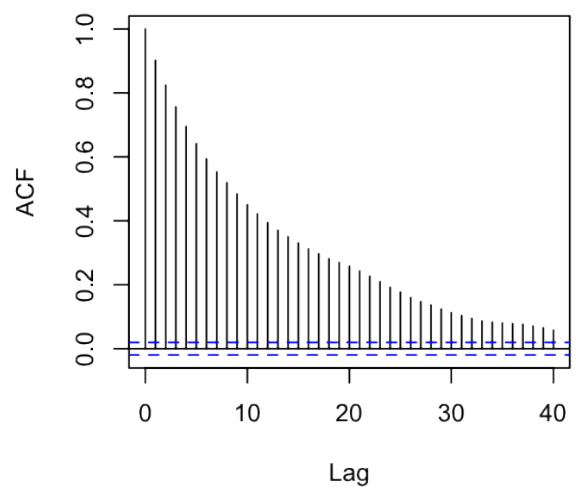
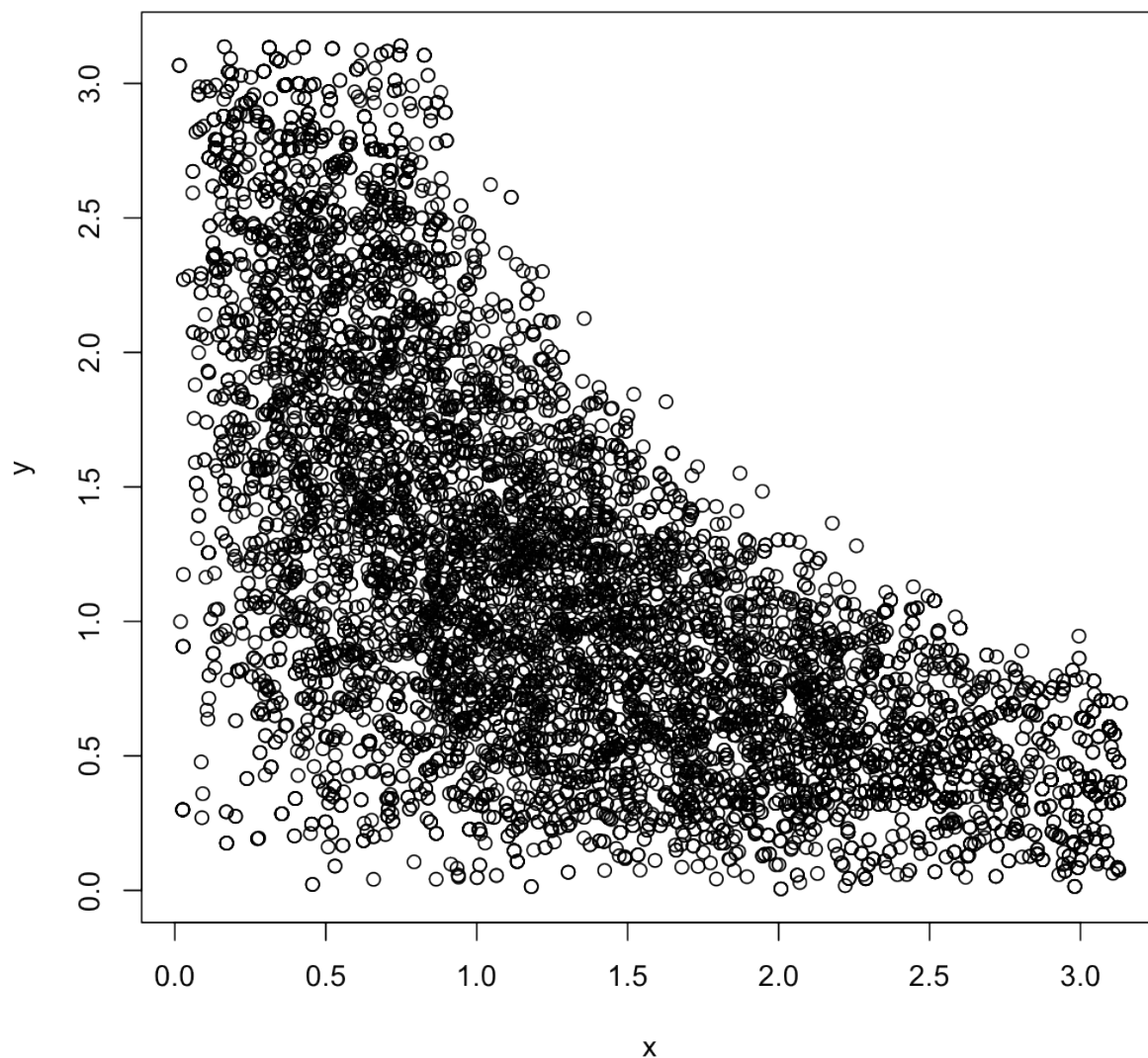**Traceplot of 1 populations**
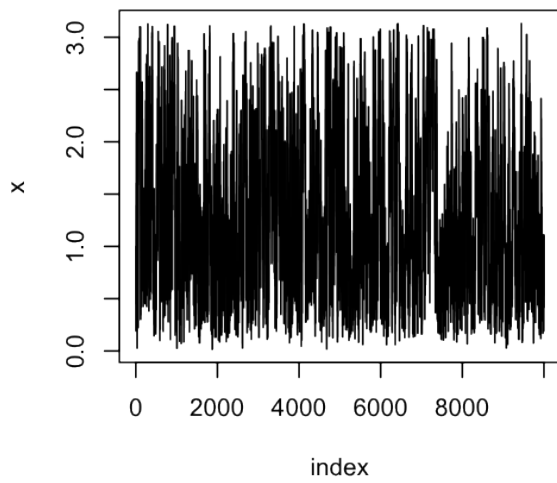
Traceplot of 1 populations

Series x

Series y

```
plot(t(simplify2array(chain2)[1, , ]))
```

3

1.2   Multiple chains in parallel

If the target density returns a vector instead of a scalar, we can run multiple chains in parallel. Our proposal updater should update the entire population. If a state is a matrix (as created here by `rbind`), then plot (*et. al.*) assumes multiple parallel chains.[3]
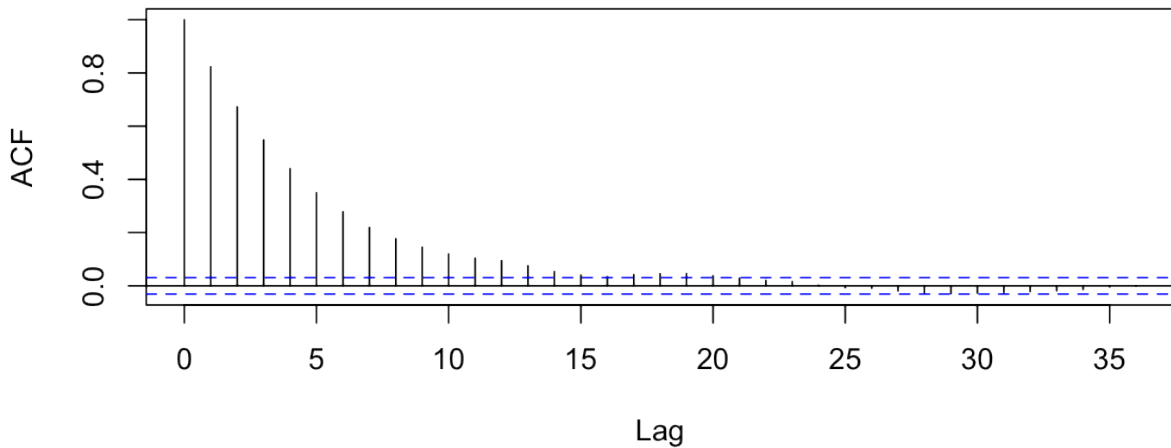
```
chain3 <- iterate(1000, updater, init = rbind(0.1, 0.5, 2.5, 3.1))
plot(chain3)
```

---

[3]The whole issue of what the "default" structure of a state is flexible at this point, and I haven't given much thought yet to what the optimal setup may be. On the todo list.

## Traceplot of 4 populations
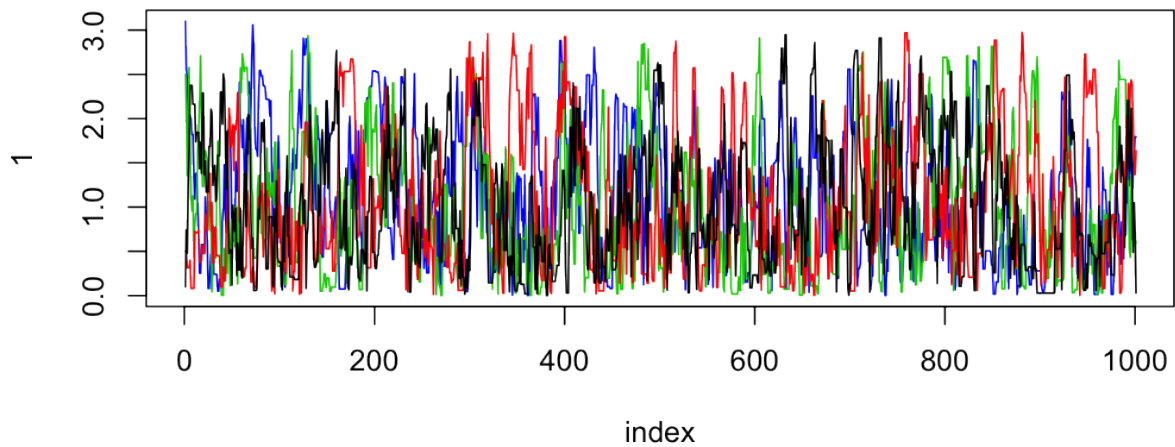
Series

Multiple chains of multivariate samples are also possible, as long as a logical vector of the same length as that returned by the density function will "correctly" subset individuals from the population state object. [4]

```
mvt2 <- function(x) apply(x, 1, mvtarget)
mvup2 <- metropolis(mvt2, propose)
init <- rbind(c(x = 1, y = 3), c(0.1, 0.5), c(1, 1))
chain4 <- iterate(10000, mvup2, init)
plot(chain4)
```

---

[4]Thus, a population can be a vector, a matrix with individuals in rows, or a list. Some convenience methods such as print, summary, plot, hist, etc., assume a population is a matrix, but this is not strictly required.

Traceplot of 3 populations

Traceplot of 3 populations

Series x

Series y
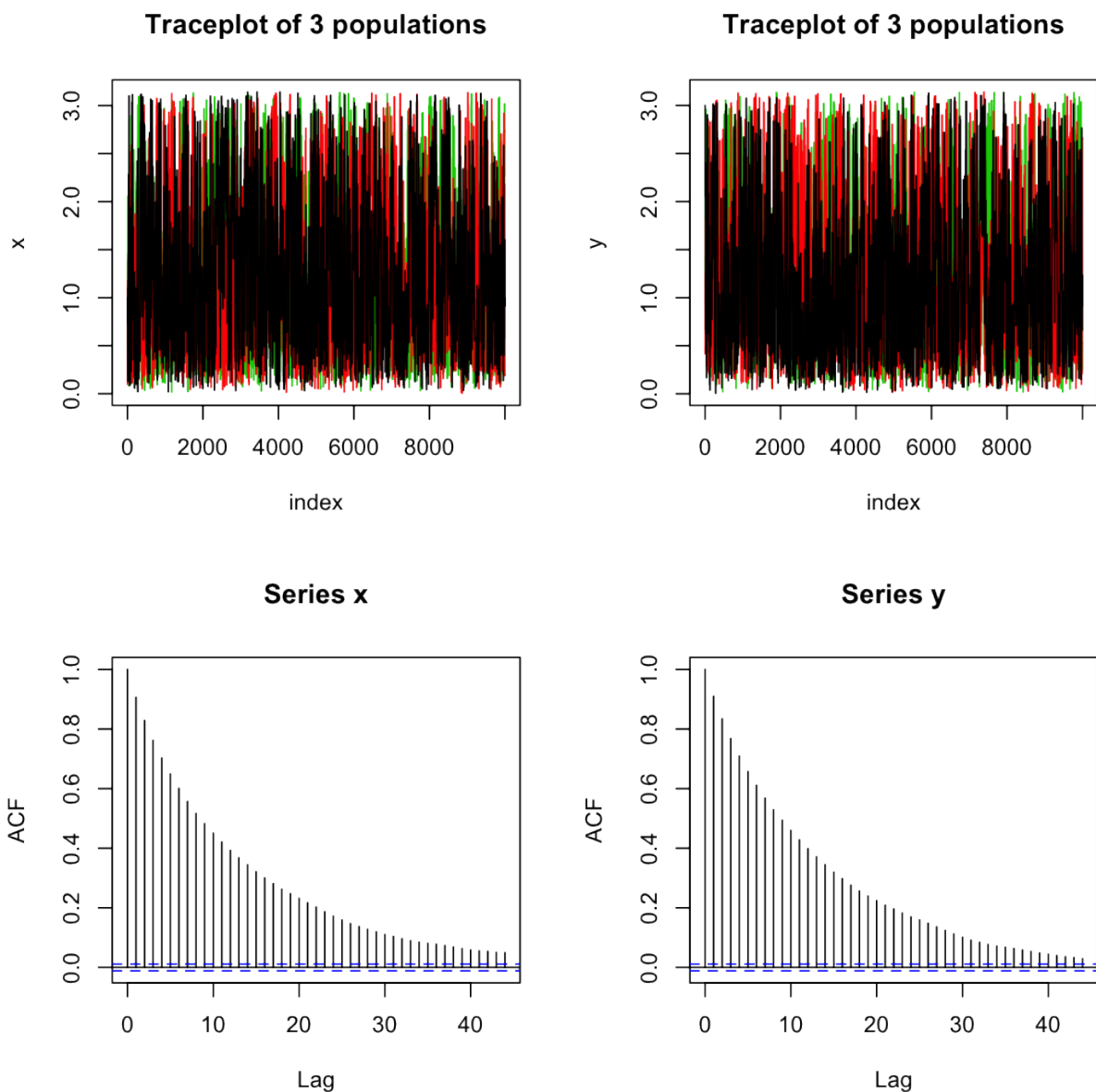
1.3   Gibbs sampling

A gibbs updater calls several updating functions sequentially. Here we find Baysean location-scale parameter estimates for a t-distribution likelihood with known degrees of freedom $5/2$. The model specification in this case is $y|\mu, w \sim N(\mu, w^{-1})$ and $w|\sigma^2, \nu \sim G(\nu/2, \sigma^2\nu/2)$, with priors $\mu \sim N$ and $\sigma^2 \sim G$.

```
newcomb <- c(28, -44, 29, 30, 26, 27, 22, 23, 33, 16, 24, 29, 24, 40, 21, 31,
    34, -2, 25, 19, 24, 28, 37, 32, 20, 25, 25, 36, 36, 21, 28, 26, 32, 28,
    26, 30, 36, 29, 30, 22, 36, 27, 26, 28, 29, 23, 31, 32, 24, 27, 27, 27,
    32, 25, 28, 27, 26, 24, 32, 29, 28, 33, 39, 25, 16, 23)
##' Full conditional updater for mu
```

```r
f.m <- function(state, ...) {
    k <- seq_len(ncol(state) - length(newcomb))
    w <- rowSums(state[, -k])
    mu <- (state[, -k] %*% newcomb)/(1e-04 + w)
    sd <- 1/sqrt(1e-04 + w)
    n <- nrow(state)
    state[, 1] <- rnorm(n, mu, sd)
    state
}
##' Full conditional updater for sigma^2
f.v <- function(state, df = FALSE) {
    nu <- if (df)
        1/state[, 3] else 5
    k <- seq_len(ncol(state) - length(newcomb))
    n <- ncol(state[, -k])
    rates <- 0.1 + rowSums(state[, -k]) * nu/2
    state[, 2] <- rgamma(nrow(state), 0.1 + n * nu/2, rates)
    state
}
##' Full conditional updater for w
f.w <- function(state, df = FALSE) {
    nu <- if (df)
        1/state[, 3] else 5
    k <- seq_len(ncol(state) - length(newcomb))
    rate <- (nu * state[, 2] + t(apply(state, 1, function(row) (newcomb - row[1])^2)))/2
    state[, -k] <- rgamma(length(state[, -k]), (nu + 1)/2, rate)
    state
}
```
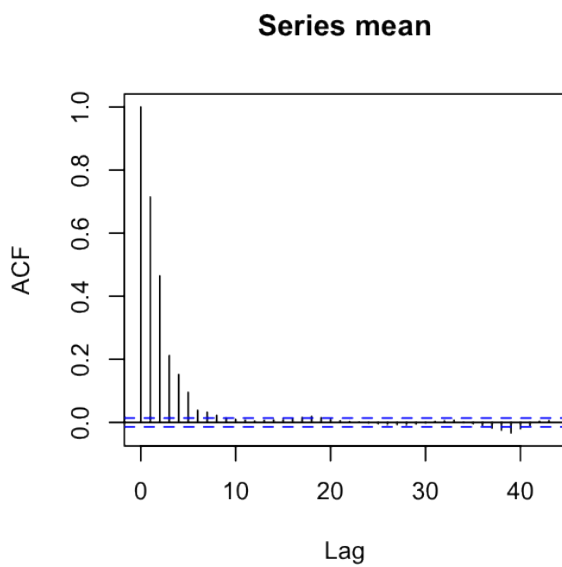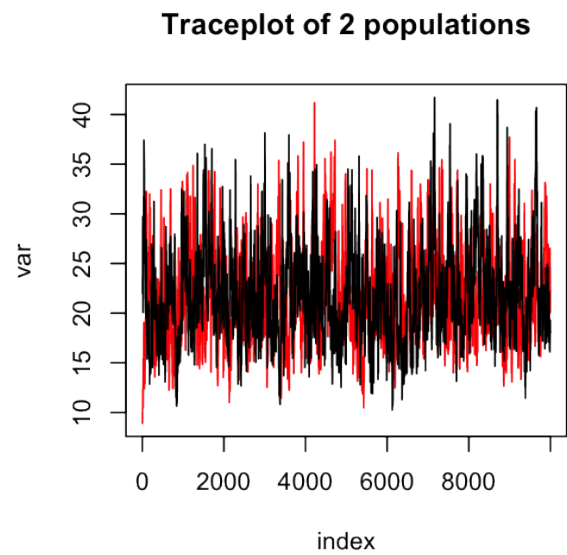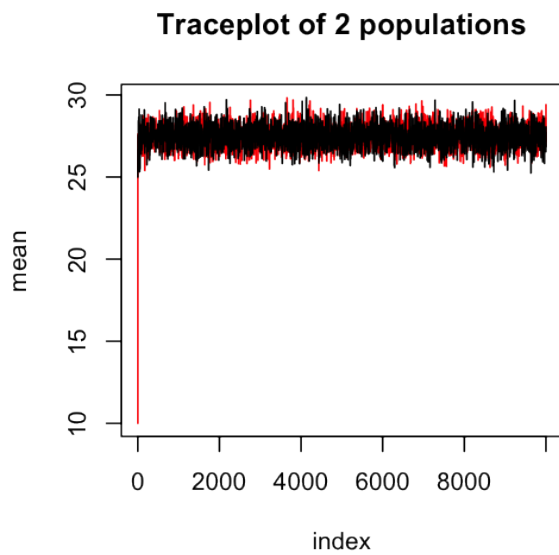
The gibbs function is used to create a function which acts as the Gibbs updater.

```r
init <- rbind(c(mean = 25, var = 22, rgamma(length(newcomb), 5/2, 22 * 5/2)),
    c(10, 10, rgamma(length(newcomb), 5/2, 10 * 5/2)))
newcomb.gibbs <- gibbs(f.m, f.v, f.w)
chain5 <- iterate(10000, newcomb.gibbs, init)
chain5 <- prune(chain5, TRUE, 1:2)
plot(chain5)
```

Traceplot of 2 populations

Traceplot of 2 populations

Series mean

Series var
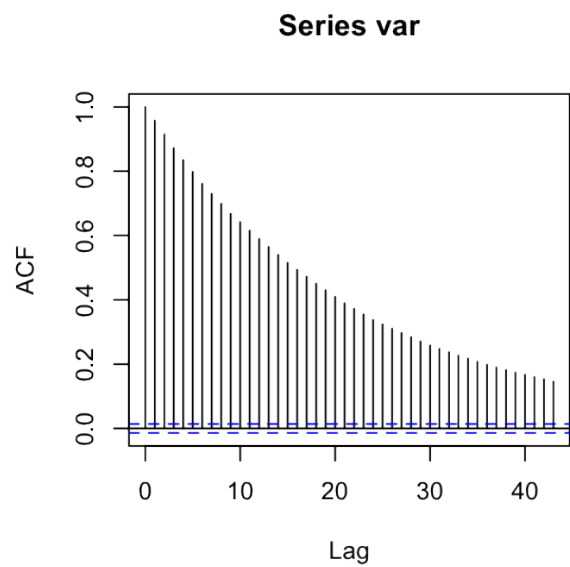

```
summary(chain5)
```

```
## Discarding first 1000 states.
##            mean       var
## mean    27.4908   21.995
## se       0.6638    4.782
## 2.5%    26.1954   14.250
## 97.5%   28.8291   33.006
```

Of course, you can use a metropolis updater in place of a full conditional. Here we put a prior on $\nu^{-1} \sim E(1)T(0,1)$
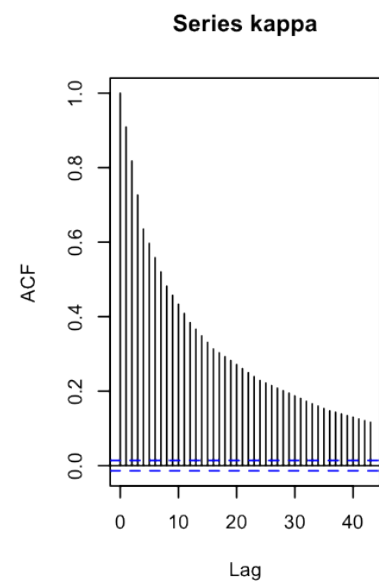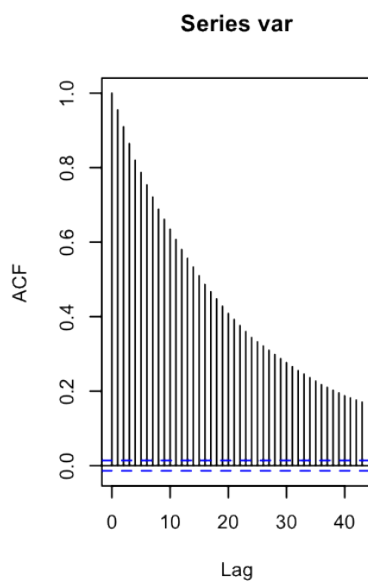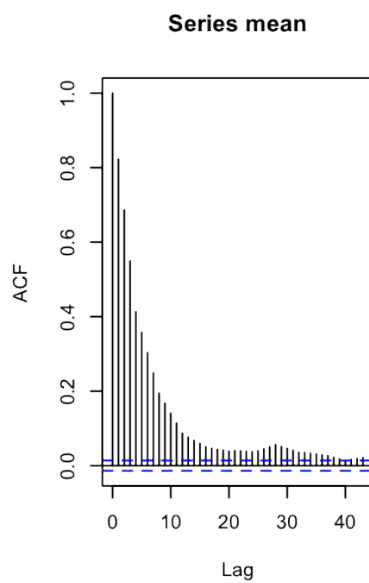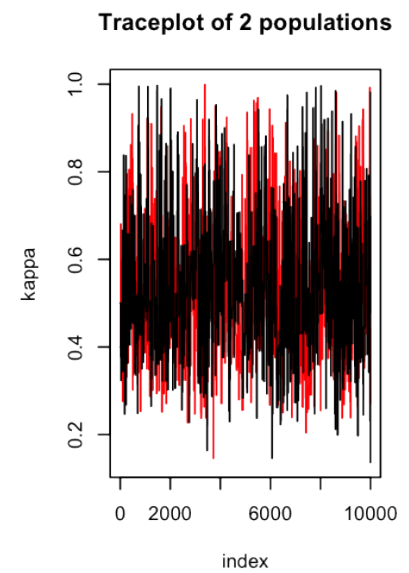
```
dtexp <- function(x, rate = 1, min = 0, max = Inf, log = FALSE) {
    d <- dexp(x, rate) * (x >= min) * (x <= max)
    c <- pexp(max, rate) - pexp(min, rate)
    if (log)
        log(d/c) else d/c
}
posterior <- function(state) {
    if (!is.matrix(state))
        state <- matrix(state, 1)
    f <- function(x) sum(dt((newcomb - x[1])/sqrt(x[2]), 1/x[3], log = TRUE) -
        log(x[2])/2)
    (apply(state, 1, f) + dnorm(state[, 1], sd = 100, log = TRUE) + dgamma(state[,
        2], 0.1, 0.1, log = TRUE) + dtexp(state[, 3], max = 1, log = TRUE))
}
kappa.prop <- function(state, ...) {
    state[, 3] <- runif(nrow(state))
    state
}
init <- rbind(c(mean = 25, var = 22, kappa = 0.5, rgamma(length(newcomb), 5/2,
    22 * 5/2)), c(10, 10, 0.4, rgamma(length(newcomb), 5/2, 10 * 5/2)))
newcomb.chain3 <- gibbs(f.m, f.v, f.w, metropolis(posterior, kappa.prop))
chain4 <- iterate(10000, newcomb.chain3, init, df = TRUE)
chain4 <- prune(chain4, TRUE, 1:3)
summary(chain4)

## Discarding first 1000 states.
##           mean    var  kappa
## mean   27.3778 13.098 0.5377
## se      0.5836  4.001 0.1495
## 2.5%   26.2392  6.868 0.2718
## 97.5%  28.5624 22.274 0.8639

plot(chain4)
```
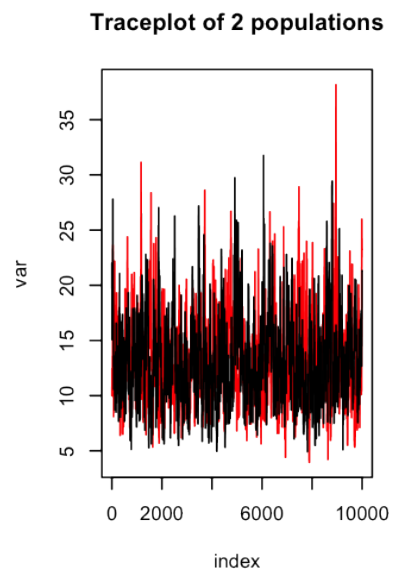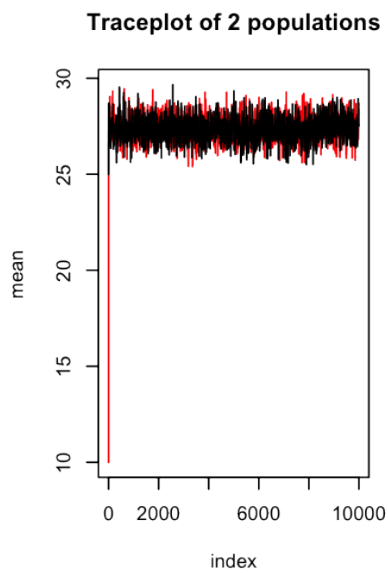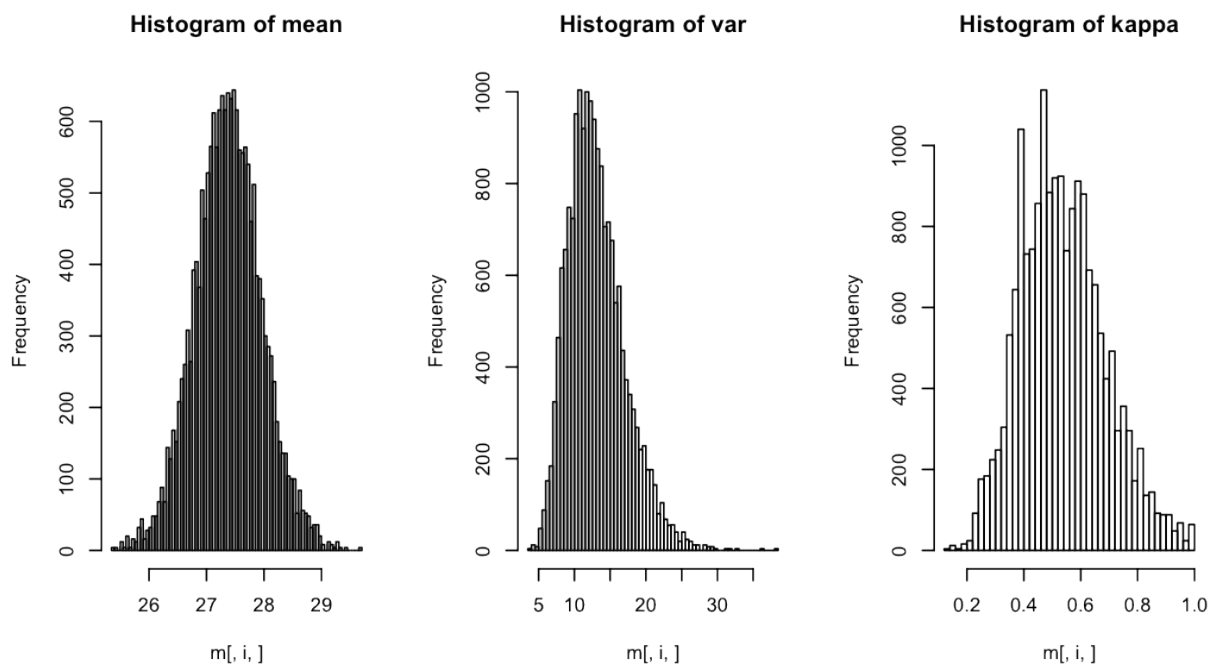
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Traceplot of 2 populations | Traceplot of 2 populations | Traceplot of 2 populations

Series mean | Series var | Series kappa


```
hist(chain4, breaks = "fd")

## Discarding first 1000 states.
```

Histogram of mean   **Histogram of var**   **Histogram of kappa**

1.4 Parallel tempering

We want to sample from a distribution with separated modes. First we set up the target distribution function. This function should take a single individual and return the density of that individual.

```
f <- function(state) log(dnorm(state) + dnorm(state, 10))
```

Now we can set up the parallel tempering updater. Function temper is similar to metropolis, but you must also provide a list of temperatures. (It is assumed that the number of individuals in the population will be the same as the number of temperature levels.)

```
temps <- c(1, 2, 4, 8, 15)
updater <- mutate(heat(f, temps), propose)
init <- rbind(-3, 0, 5, 10, 15)
gch <- iterate(10000, updater, init)
plot(gch)
```
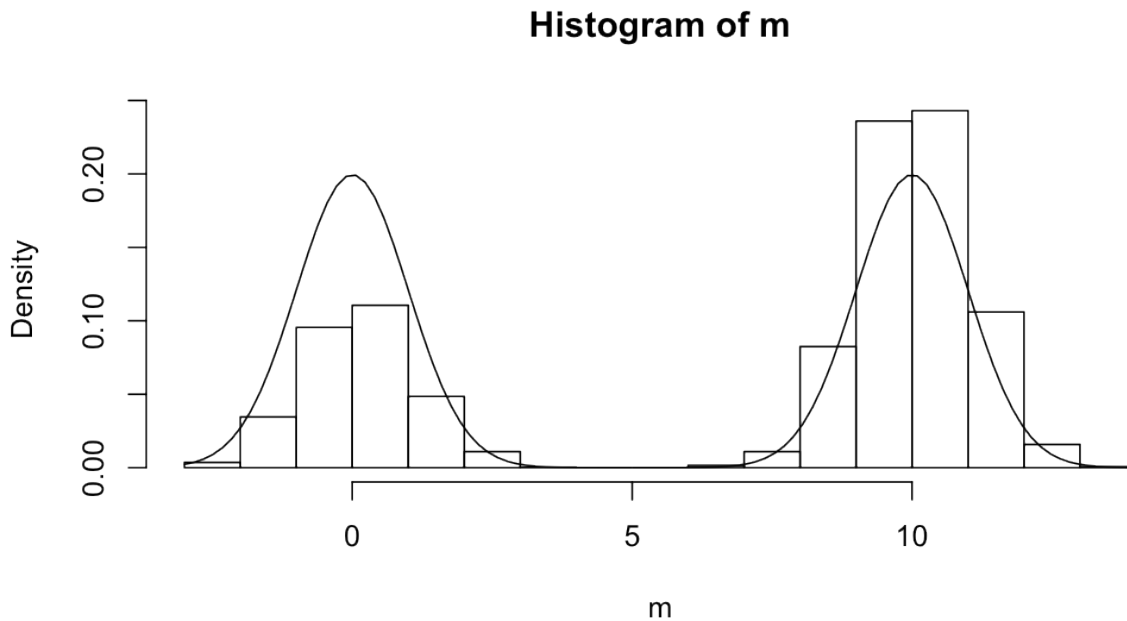
Traceplot of 5 populations
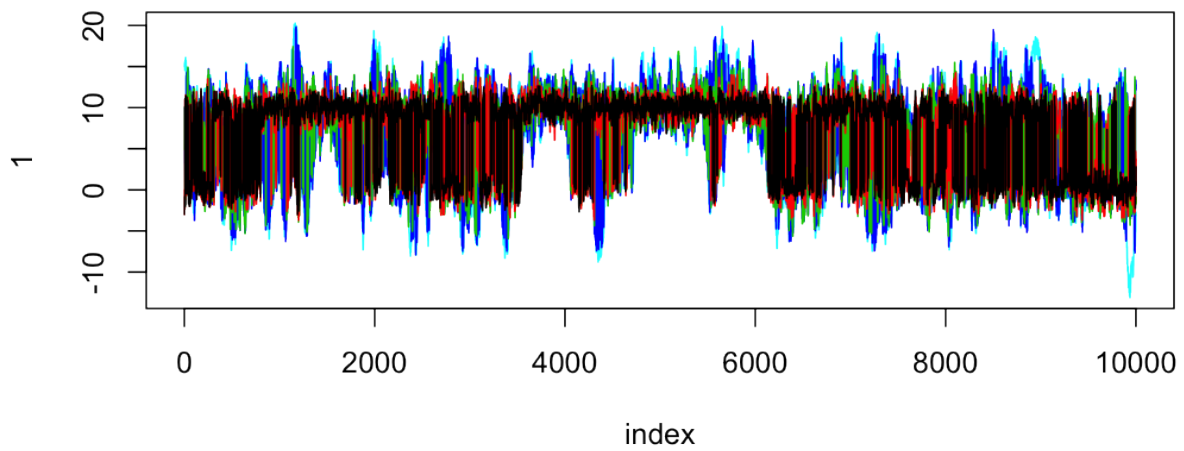
Series
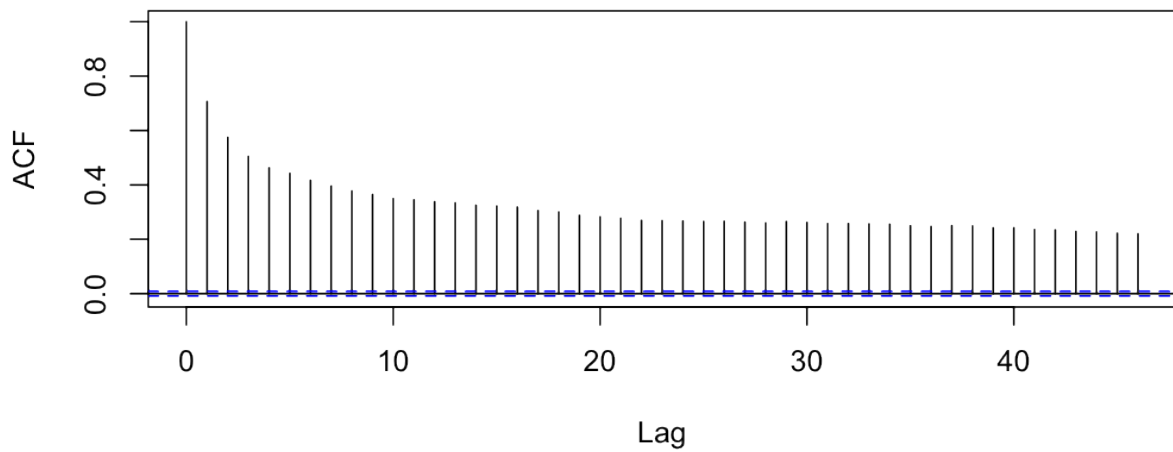

```
xx <- prune(gch, 1, 1)  #extract chain with correct distribution
```

```
hist(xx, freq = FALSE, breaks = "fd")

## Discarding first 1000 states.

curve((dnorm(x) + dnorm(x, 10))/2, add = TRUE)
```

Histogram of m

1.5 Evolutionary MC

Here we go with the real-deal. Twenty part trivariate-gaussian mixure. The target function is a part of the evolMC package.

```
means <- t(replicate(20, runif(3, -10, 10)))
dmix <- function(x) target(x, means)
ladder <- heat(dmix, temps)
e <- seq(0.2, 3, length = 5)
runif3 <- function(x) x + runif(length(x), -e, e)
runif4 <- function(x) x + rnorm(length(x), 0, 0.25 * temps)
evolve <- gibbs(reproduce(ladder), mutate(ladder, runif4), p = c(1, 1))
ptemp <- mutate(ladder, runif4)
wt.evolve <- gibbs(weighted.reproduce(ladder), mutate(ladder, runif4), p = c(1,
    1))

init <- matrix(0, 5, 3)
# invisible(runif(100)) lineage <- iterate(2000, evolve, init, bar=1)
# pt.lineage <- iterate(2000, ptemp, init, bar=1)
wt.lineage <- iterate(2000, wt.evolve, init, bar = 1)

## ==========================================================================


plot(lineage)
```
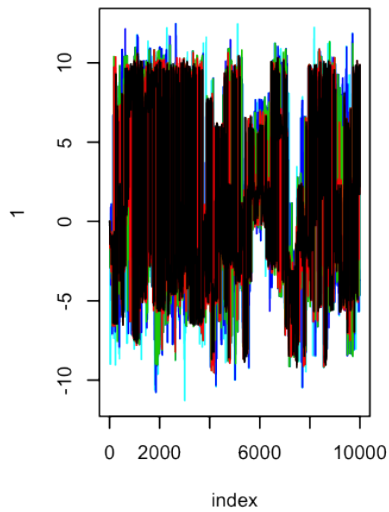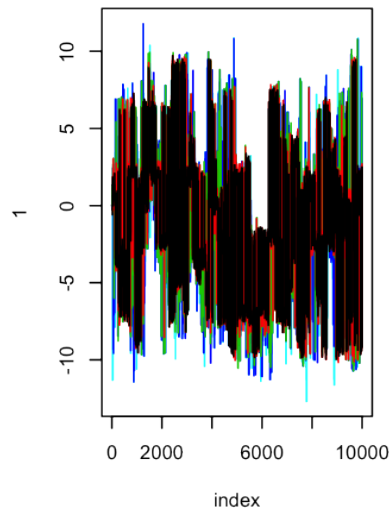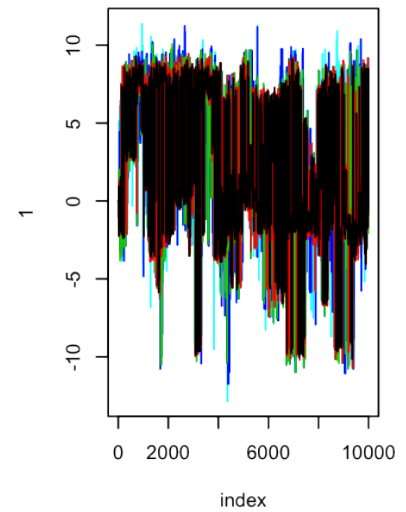
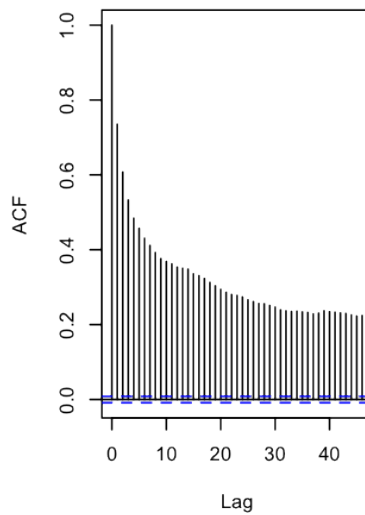**Traceplot of 5 populations**   **Traceplot of 5 populations**   **Traceplot of 5 populations**
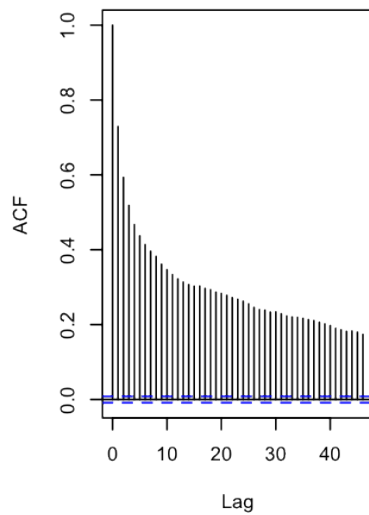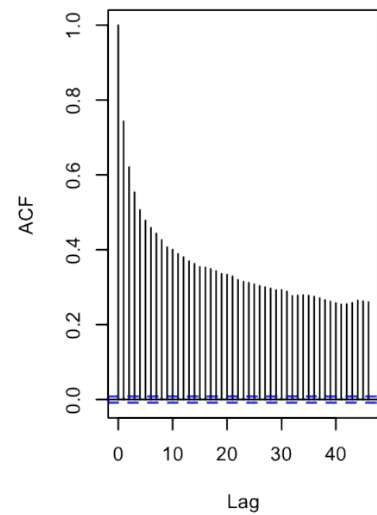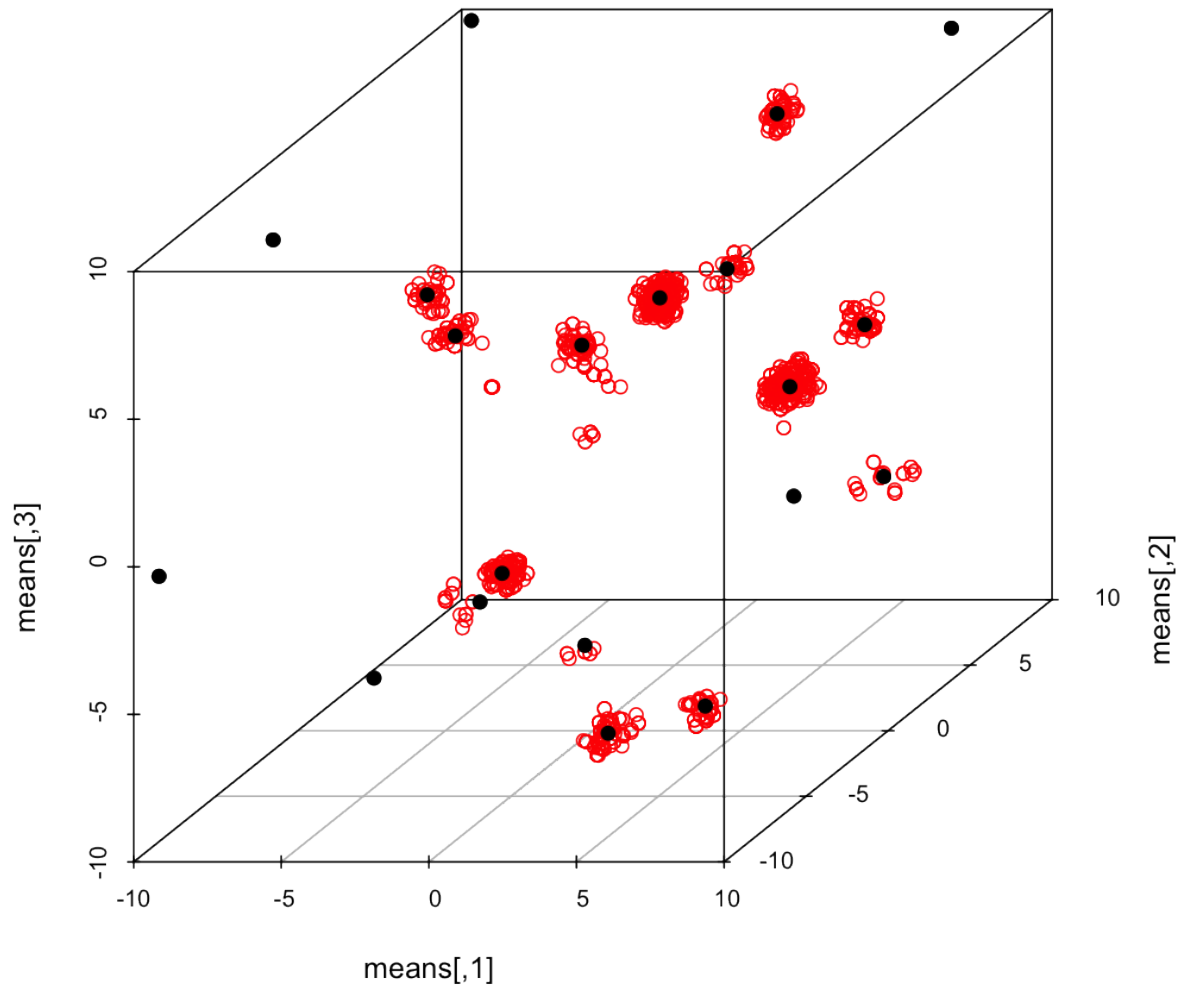
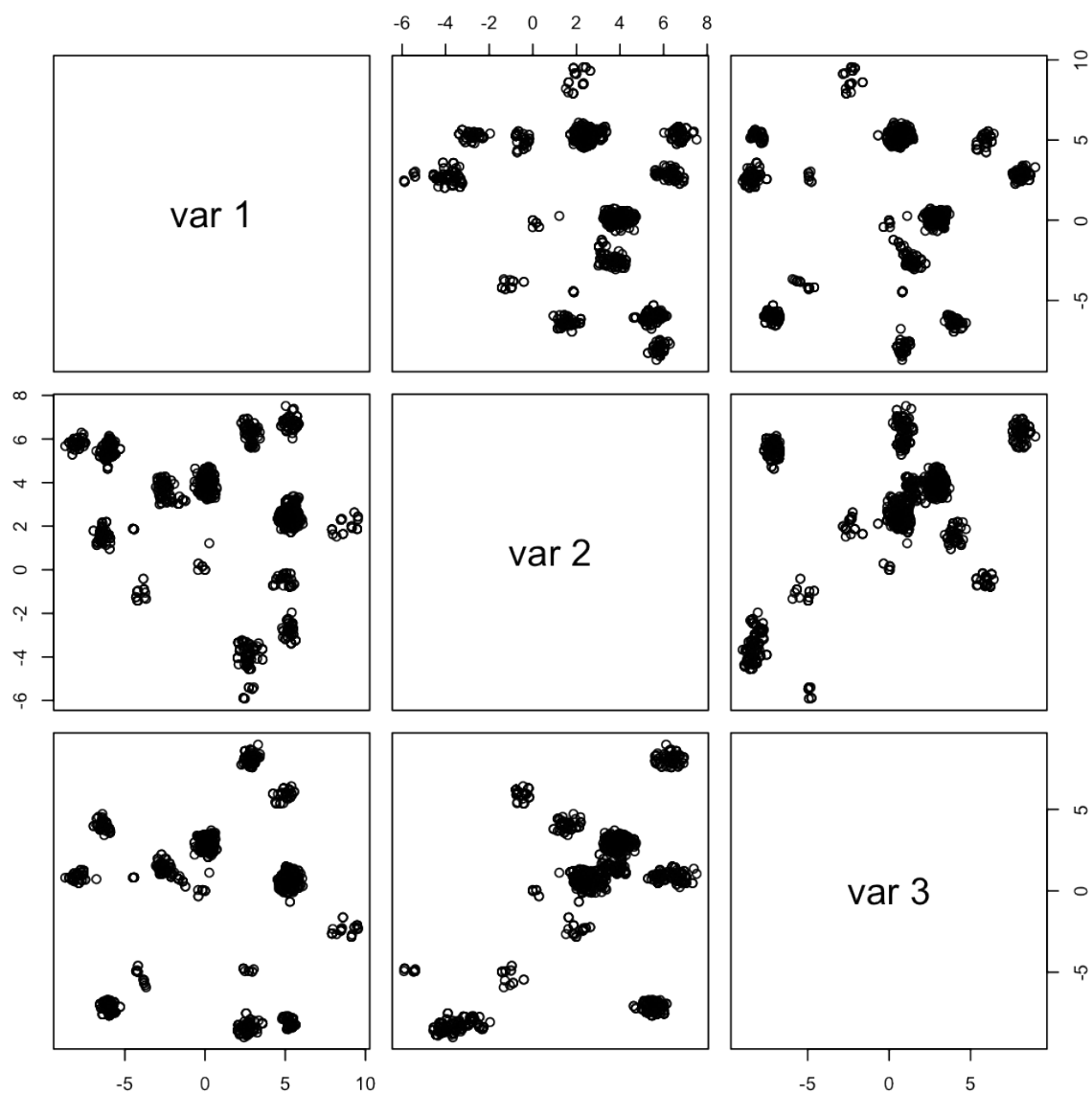**Series**   **Series**   **Series**

```r
m <- aperm(simplify2array(wt.lineage))
## wt.m <- aperm(simplify2array(wt.lineage)) pt.m <-
## aperm(simplify2array(pt.lineage))
library(scatterplot3d)
pp <- scatterplot3d(means)
# invisible(sapply(5:1,function(i) pp£points3d(m[,,i],col=i+1)))
pp$points3d(m[, , 1], col = 2)
## pp£points3d(wt.m[,,1],col=3) pp£points3d(pt.m[,,1],col=3)
## pp£points3d(m[,,1],col=2)

pp$points3d(means, col = 1, pch = 19)
```

```
pairs(m[, , 1])
```

```
## library(rgl) plot3d(m[,,1]) plot3d(means,pch=19,size=15)
## sapply(1:5,function(i) points3d(m[,,i],col=i+1))
```