OxWaSP Module 1: Adaptive MCMC draft

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1 Introduction to Adaptive MCMC - the AM algorithm

MCMC algorithms allow sampling from complicated, high-dimensional distributions. Choice of the proposal distribution (from which samples are taken in an attempt to approximate sampling from the target distribution π) determines the ability of the algorithm to explore the parameter space fully and hence draw a good sample. Adaptive MCMC algorithms tackle this challenge by using samples already generated to learn about the target distribution; they push this knowledge back to the choice of proposal distribution iteratively.

This project explores adaptive MCMC algorithms existing in the literature that use covariance estimators to improve convergence to a target distribution supported on a subset of $\mathbb{R}^d$. In this schema we learn about the target distribution π through estimation of its correlation structure from the MCMC samples. We use this correlation structure to improve our estimate of the target.

We first implement an adaptive MCMC algorithm AM (Haario et al., 2001) which is a modification of the random walk Metropolis-Hastings algorithm. In AM the proposal distribution is updated at time t to be a normal distribution centered on the current point X_{t-1} with covariance $C_t(X_0, ..., X_{t-1})$ that depends on the the whole history of the chain. The use of historic states means the resulting chain is non-markovian, and reversibility conditions are not satisfied. Haario et al show that, with a small update to the usual Metropolis-Hastings acceptance probability, the right ergodic properties and correct simulation of the target distribution none the less remain. The probability with which to accept candidate points in the chain becomes:

$$\alpha(X_{t-1}, Y) = \min\left(1, \frac{\pi(Y)}{\pi(X_{t-1})}\right)$$

With C_t given by:

$$C_t = s_d \text{cov}(X_0, ..., X_{t-1}) + s_d \epsilon I_d$$

Here cov() is the usual empirical covariance matrix, and the parameter $s_d = \frac{2.4^2}{d}$ (Gelman et al., 1996). ϵ is chosen to be very small compared to the subset of $\mathbb{R}^d$ upon which the target function is supported. The AM algorithm is computationally feasible due to recursive updating of the covariance matrix on acquisition of each new sample through the relation:

$$C_{t+1} = \frac{t-1}{t}C_t + \frac{s_d}{t}(t\bar{X}_{t-1}\bar{X}_{t-1}^T - (t+1)\bar{X}_t\bar{X}_t^T + X_tX_t^T + \epsilon I_d)$$

with the mean calculated recursively by:

$$\bar{X}_{t+1} = \frac{t\bar{X}_t + X_{t+1}}{t+1}$$

Because of the instability of the covariance matrix, to implement the adaptivity we first run the algorithm with no change to the covariance of the proposal distribution. The adaptation starts at a user defined point in time, and until this time the covariance of the proposal is chosen to represent our best knowledge of the target distribution.

2 An example - testing the AM algorithm

We now numerically test the AM algorithm. We have used two different target distributions: a correlated Gaussian distribution $N(0, \Sigma)$ and a "banana"-shaped distribution ((Roberts and Rosenthal, 2009)) given by:

$$f_B(x_1, ..., x_d) \propto \exp\left[-x_1^2/200 - \frac{1}{2}\left(x_2 + Bx_1^2 - 100B\right)^2 - \frac{1}{2}\left(x_3^2 + x_4^2 + ... + x_d^2\right)\right]$$

$B > 0$ is the "bananicty" constant (set to 0.1 throughout) and d is the dimension. We have chosen the correlated Guassian distribution as targetting this demonstrates how the use of empirical covariance improves convergence - we learn the target's covariance as we move through steps of the MCMC. The banana-shaped distribution is an additional example with an irregular shape. We use this to test the ability of the markov chain to fully explore the state space with and without adaption. We first run our implementation of the AM algorithm targetting $N(0, \Sigma)$ with

```
d = 8
n_iter = 200     #  Total number of iterations
x_1 = rep(5,d)       #  Vector of inital values
t_adapt = 50      #  When to start adapting
adapt = "None"       #  Choose the type of adaptation.

X_MH = mcmc(target = pi_norm_corr,
         n_iter = n_iter,
         x_1 = x_1,
         adapt=adapt)
```

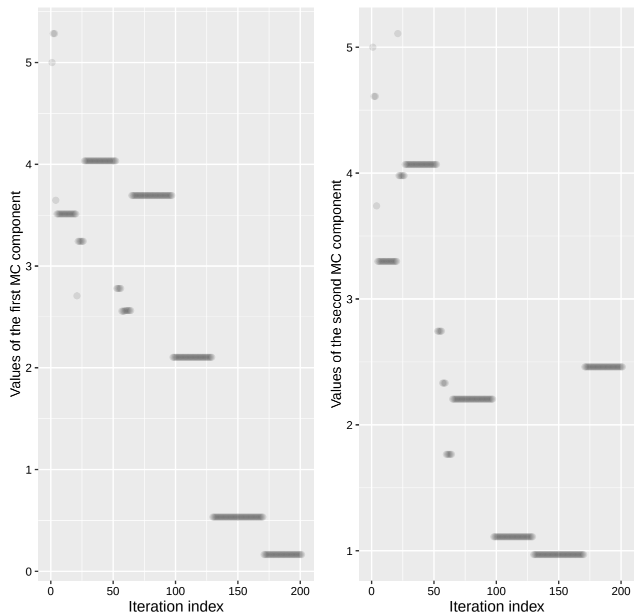


Figure 1: This is the first graph

```
## Running MCMC targeting  pi_norm_corr with  200 iterations.
## Adaptation algorithm is:  None .
## Covariance matrix estimator is:  Sample covariance .
## MCMC finished in 0.1159534 seconds.
## The last acceptance rate was: 0.065
```

```
adapt = "AM"       #  Choose the type of adaptation.
cov_estimator="Sample covariance"    #  Choose the type of covariance matrix estimator.

X_AM = mcmc(target = pi_norm_corr,
         n_iter = n_iter,
         x_1 = x_1,
         adapt=adapt,
         t_adapt = t_adapt,
         cov_estimator=cov_estimator
         )
```

```
## Running MCMC targeting  pi_norm_corr with  200 iterations.
## Adaptation algorithm is:  AM .
## Covariance matrix estimator is:  Sample covariance .
## MCMC finished in 1.991497 seconds.
```

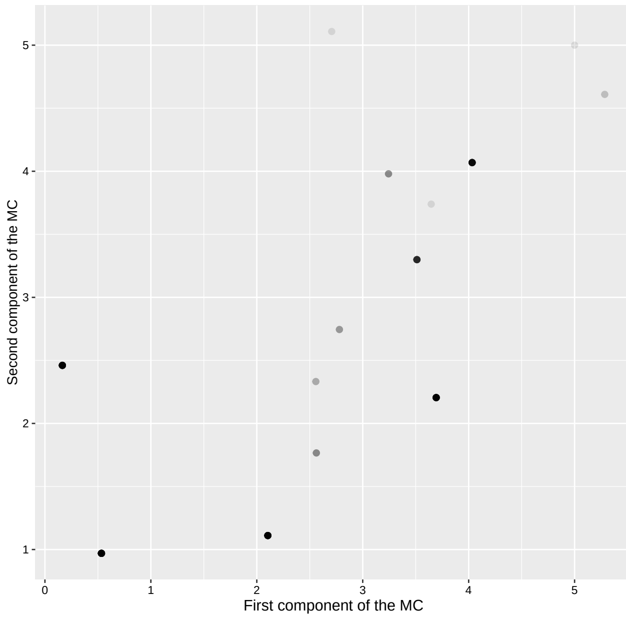


Figure 2: This is the first graph

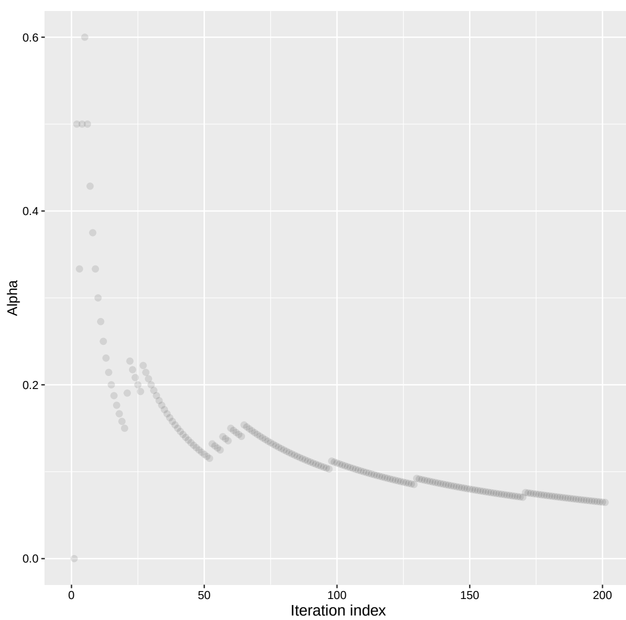


Figure 3: This is the first graph

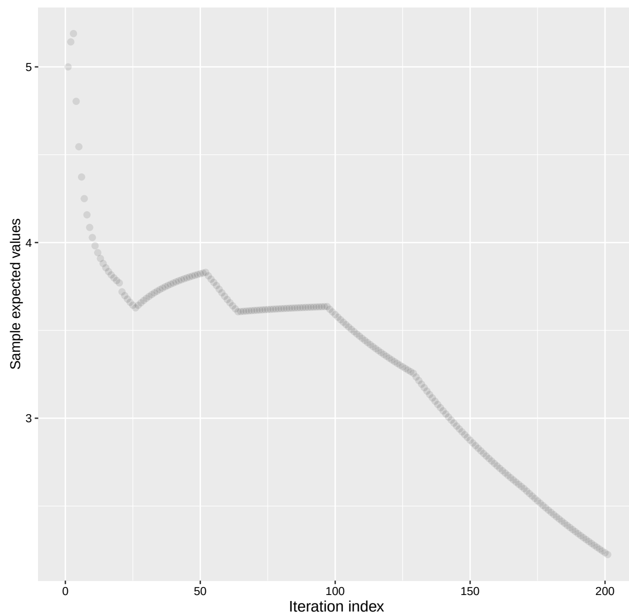
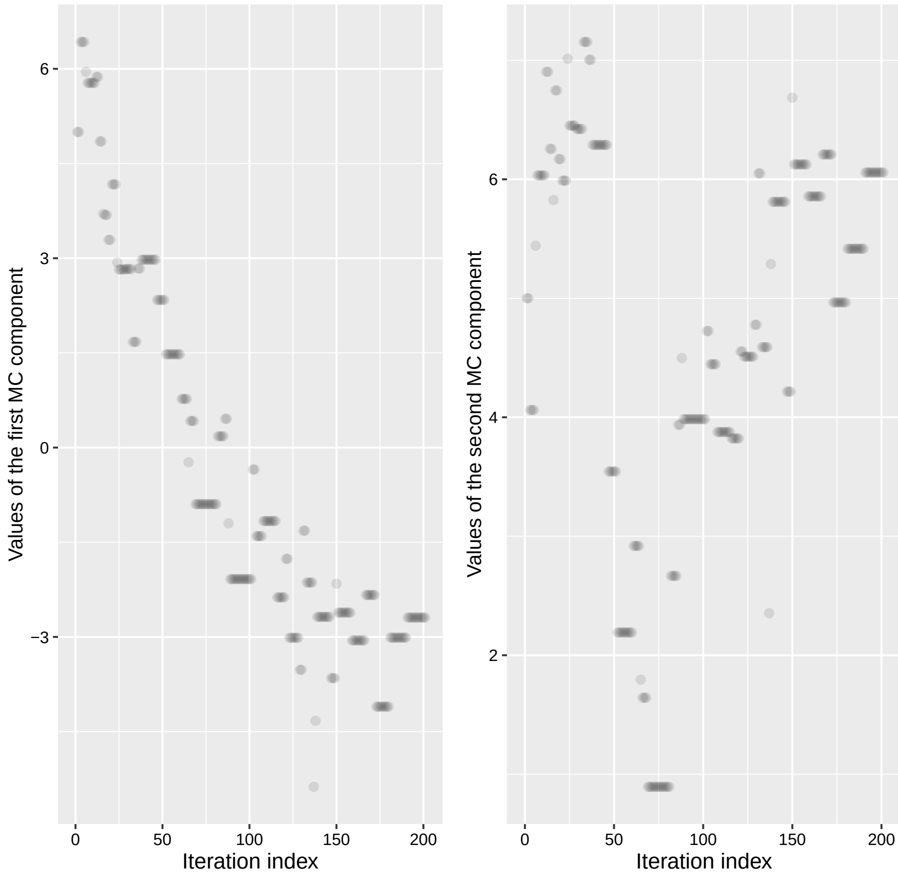
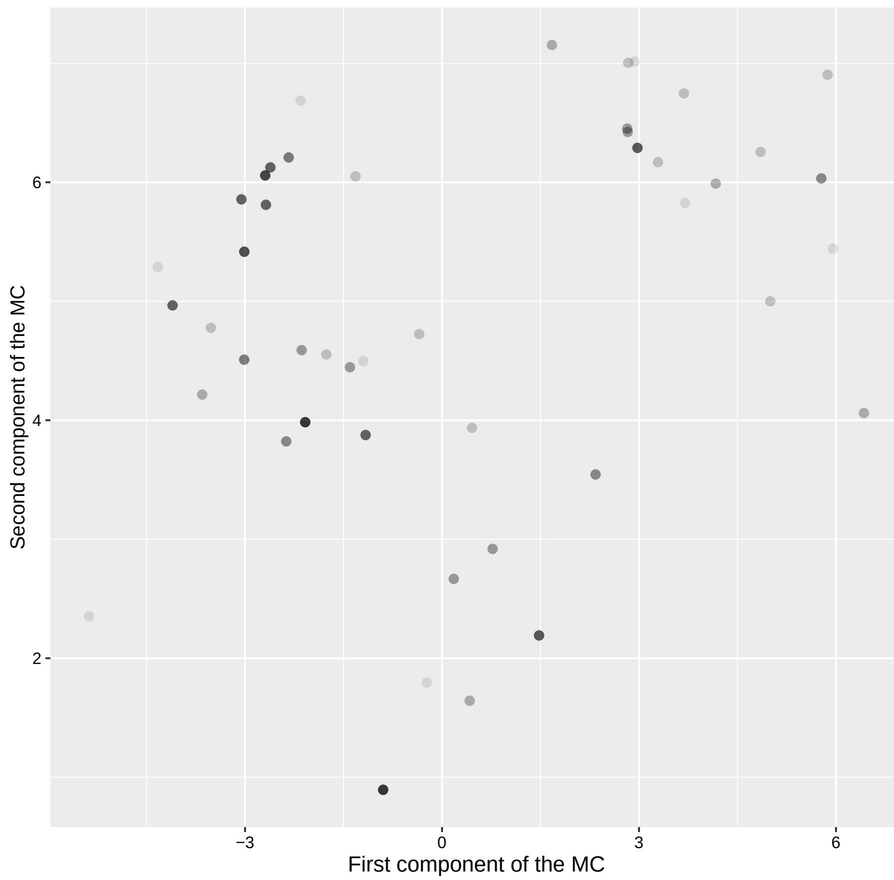


Figure 4: This is the first graph

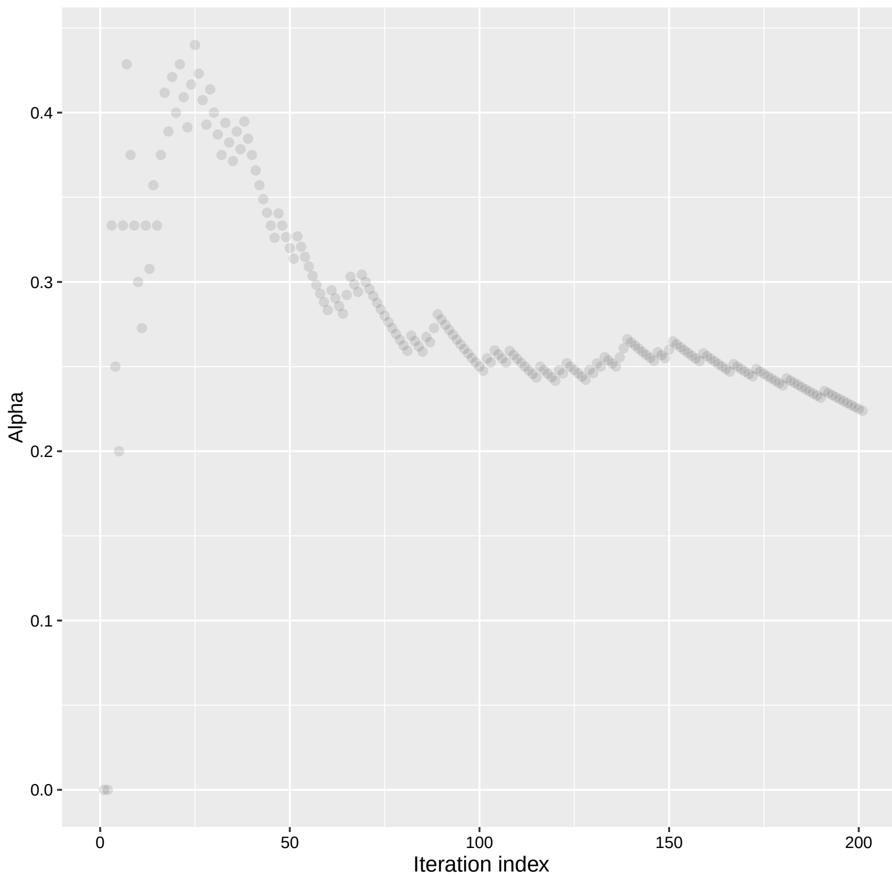
```
## The last acceptance rate was: 0.225

plot6=plotIterations(
                    X_AM$X[,1],
                    n_iter,
                    title="Values of the first MC component"
                    )
plot7=plotIterations(
                    X_AM$X[,2],
                    n_iter,
                    title="Values of the second MC component"
                    )
grid.arrange(plot6, plot7, ncol=2)
```



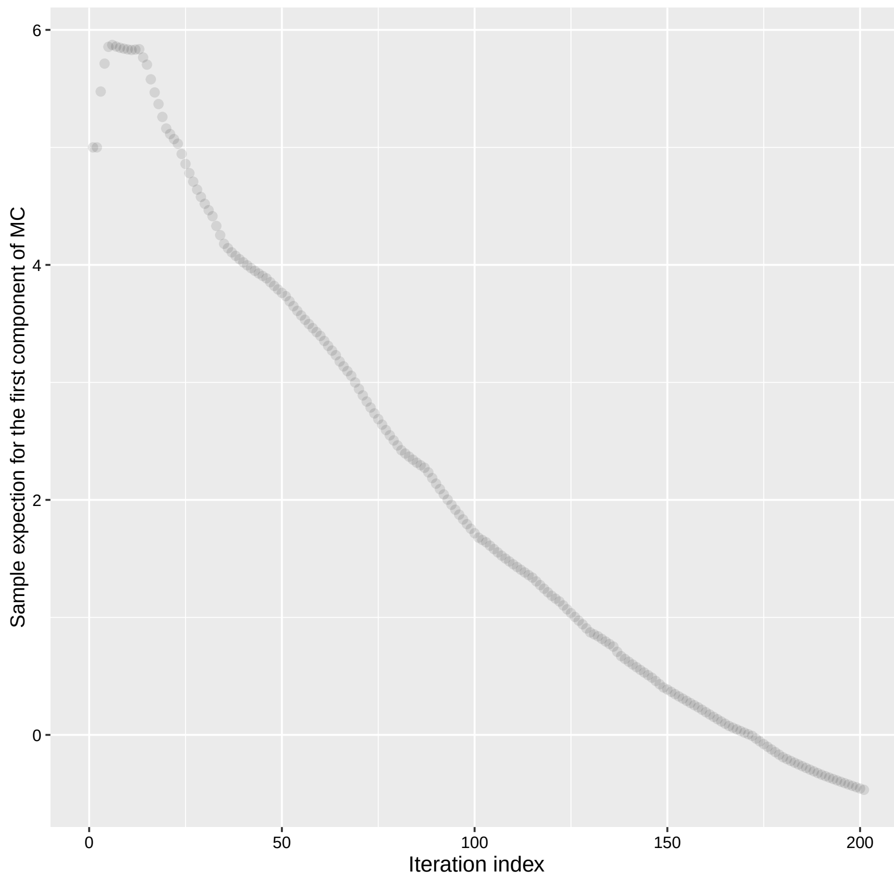

```
plot8=plotComponents(
                    X_AM$X[,1],
                    X_AM$X[,2],
                    Xtitle = "First component of the MC",
                    Ytitle = "Second component of the MC"
                    )
plot8
```




```
plot9=plotIterations(X_AM$acceptance_rates, n_iter, "Alpha")
plot9
```



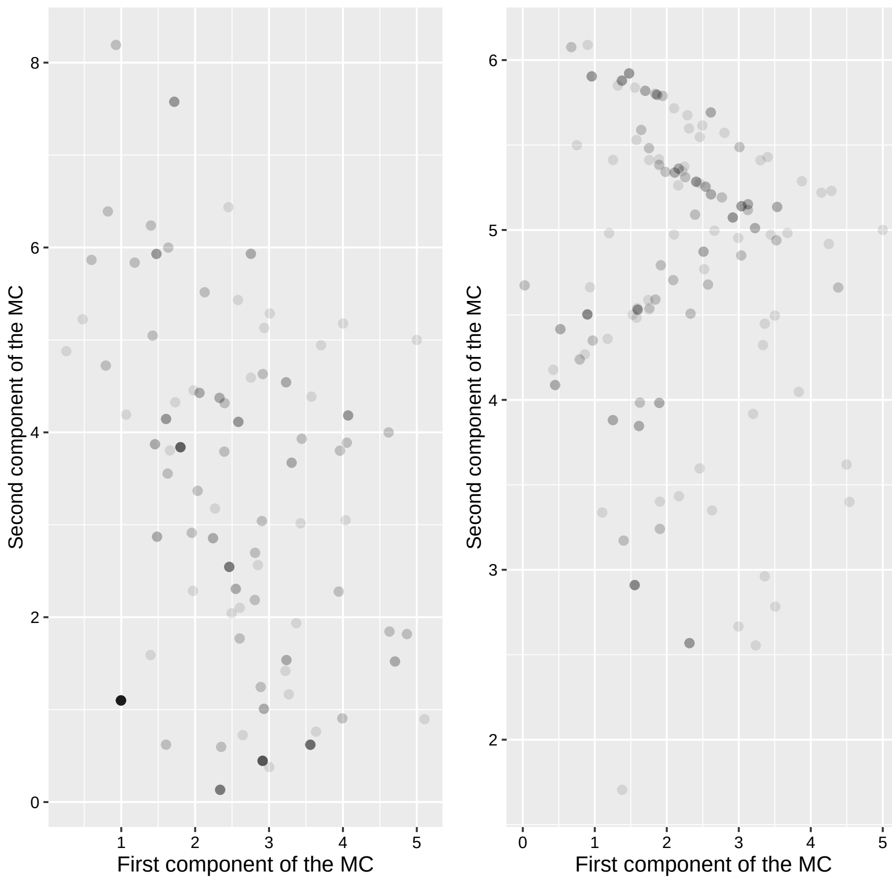

```
plot10=plotIterations(X_AM$sample_mean[,1], n_iter, "Sample expection for the first componen
plot10
```



AM is able to explore the state space, adapt properly and settle down to rapid mixing. We see an improved acceptance rate.

```
x_1 = rep(5,2)       #  Vector of inital values
target = pi_banana


X_MH_banana = mcmc(target = target,
         n_iter = n_iter,
         x_1 = x_1,
         adapt="None"
         )

## Running MCMC targeting  target with  200 iterations.
## Adaptation algorithm is:  None .
## Covariance matrix estimator is:  Sample covariance .
## MCMC finished in 0.05514789 seconds.
```

```
## The last acceptance rate was: 0.41

plot11=plotComponents(
                    X_MH_banana$X[,2],
                    X_MH_banana$X[,1],
                    Xtitle = "First component of the MC",
                    Ytitle = "Second component of the MC"
                    )

X_AM_banana = mcmc(target = target,
         n_iter = n_iter,
         x_1 = x_1,
         t_adapt = t_adapt,
         adapt="AM"
         )

## Running MCMC targeting  target with  200 iterations.
## Adaptation algorithm is:  AM .
## Covariance matrix estimator is:  Sample covariance .
## MCMC finished in 1.81484 seconds.
## The last acceptance rate was: 0.55

plot12=plotComponents(
                    X_AM_banana$X[,2],
                    X_AM_banana$X[,1],
                    Xtitle = "First component of the MC",
                    Ytitle = "Second component of the MC"
                    )
grid.arrange(plot11, plot12, ncol=2)
```



We now explore a slight modification to the adaptation scheme AM2(Roberts and Rosenthal, 2009), that uses stochastic stabilisation rather than the numerical stabilisation of AM. Roberts and Rosenthal use a mixture of Gaussians as the proposal distribution: with proportion β a normal uncorrelated distribution is mixed with a correlated normal distribution.

$$Q_n(x, \cdot) = (1-\beta)N(x, s_d\Sigma_n) + \beta(N(x, (0.1^2)I_d/d)$$

TODO Discuss the problems with starting dimension here.

```
x_1 = rep(5,8)       #  Vector of inital values
target = pi_banana8


X_AM2_banana = mcmc(target = target,
         n_iter = n_iter,
         x_1 = x_1,
```

```
         adapt="AM2"
         )

## Running MCMC targeting  target with  200 iterations.
## Adaptation algorithm is:  AM2 .
## Covariance matrix estimator is:  Sample covariance .
## MCMC finished in 0.09361219 seconds.
## The last acceptance rate was: 0.22

plot13=plotIterations(
                    X_AM_banana$X[,1],
                    n_iter,
                    title="Values of the first MC component"
                    )
plot14=plotIterations(
                    X_AM2_banana$X[,1],
                    n_iter,
                    title="Values of the first MC component"
                    )

grid.arrange(plot13, plot14, ncol=2)
```

```
x_1 = rep(5,8)      #  Vector of inital values
cov_estimator1="Shrinkage estimator"
cov_estimator2="Thresholding estimator"
target = pi_banana8

X_MH_banana = mcmc(target = target,
         n_iter = n_iter,
         x_1 = x_1,
         adapt="None"
         )

## Running MCMC targeting  target with  200 iterations.
## Adaptation algorithm is:  None .
## Covariance matrix estimator is:  Sample covariance .
## MCMC finished in 0.1331832 seconds.
## The last acceptance rate was: 0.055

X_AM_banana = mcmc(target = target,
         n_iter = n_iter,
         x_1 = x_1,
         t_adapt = t_adapt,
         adapt="AM"
         )
```

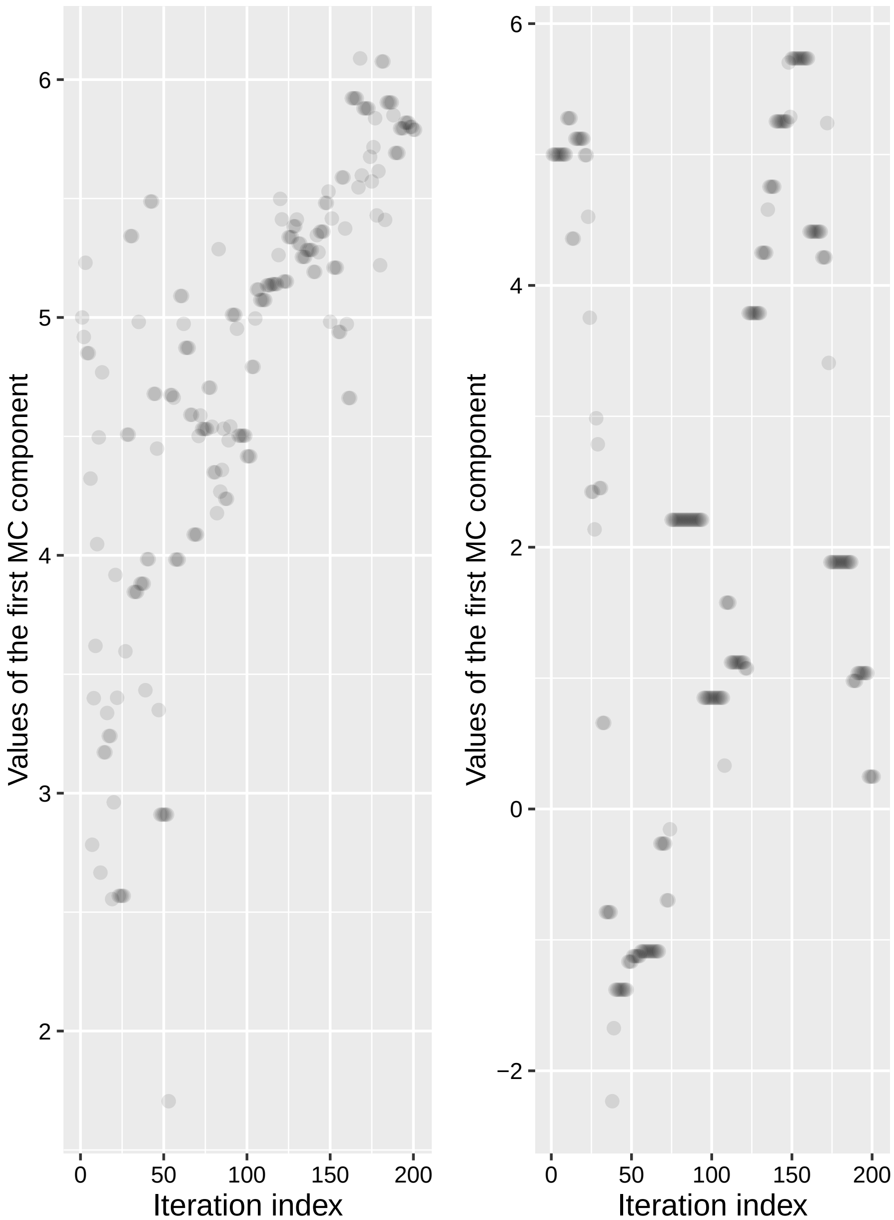


Figure 5: The first component of the 8-dimensional banana shaped distribution targetted using AM (left) and AM2 (right).

```
## Running MCMC targeting  target with  200 iterations.
## Adaptation algorithm is:  AM .
## Covariance matrix estimator is:  Sample covariance .
## MCMC finished in 1.923625 seconds.
## The last acceptance rate was: 0.195
```

```
X_AM_banana_sh= mcmc(target = target,
         n_iter = n_iter,
         x_1 = x_1,
         adapt="AM",
         t_adapt = t_adapt,
         cov_estimator=cov_estimator1
         )
```

```
## Running MCMC targeting  target with  200 iterations.
## Adaptation algorithm is:  AM .
## Covariance matrix estimator is:  Shrinkage estimator .Estimating optimal shrinkage intens
##
##
## MCMC finished in 2.394961 seconds.
## The last acceptance rate was: 0.24
```

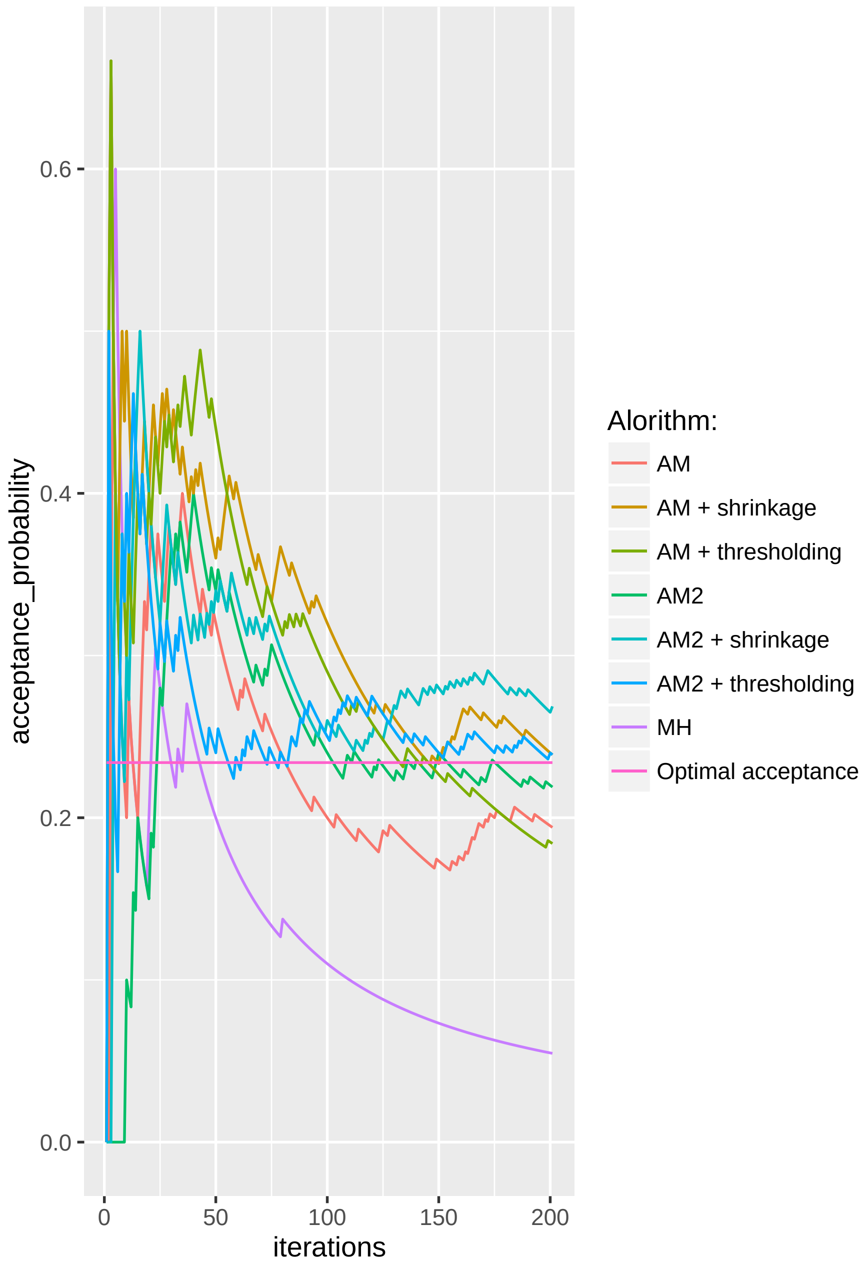
```
X_AM2_banana_sh = mcmc(target = target,
         n_iter = n_iter,
         x_1 = x_1,
         adapt="AM2",
         cov_estimator=cov_estimator1
         )
```

```
## Running MCMC targeting  target with  200 iterations.
## Adaptation algorithm is:  AM2 .
## Covariance matrix estimator is:  Shrinkage estimator .
## MCMC finished in 0.03251004 seconds.
## The last acceptance rate was: 0.265
```

```
X_AM_banana_th= mcmc(target = target,
         n_iter = n_iter,
         x_1 = x_1,
         adapt="AM",
         t_adapt = t_adapt,
         cov_estimator=cov_estimator2
         )
```

```
## Running MCMC targeting  target with  200 iterations.
## Adaptation algorithm is:  AM .
## Covariance matrix estimator is:  Thresholding estimator .
## MCMC finished in 0.2317472 seconds.
## The last acceptance rate was: 0.185
```

```
X_AM2_banana_th = mcmc(target = target,
         n_iter = n_iter,
         x_1 = x_1,
         adapt="AM2",
         cov_estimator=cov_estimator2
         )

## Running MCMC targeting  target with  200 iterations.
## Adaptation algorithm is:  AM2 .
## Covariance matrix estimator is:  Thresholding estimator .
## MCMC finished in 0.02836394 seconds.
## The last acceptance rate was: 0.24

iteration=seq(from= 1, to=n_iter+1, by=1)
#data=data.frame(iteration_count=iteration, am_alpha=X_AM_banana_sh£acceptance_rates)


df1<-data.frame(iterations=iteration,acceptance_probability=X_MH_banana$acceptance_rates)
df2<-data.frame(iterations=iteration,acceptance_probability=X_AM_banana$acceptance_rates)
df3<-data.frame(iterations=iteration,acceptance_probability=X_AM2_banana$acceptance_rates)
df4<-data.frame(iterations=iteration,acceptance_probability=X_AM_banana_sh$acceptance_rates)
df5<-data.frame(iterations=iteration,acceptance_probability=X_AM2_banana_sh$acceptance_rates
df6<-data.frame(iterations=iteration,acceptance_probability=X_AM_banana_th$acceptance_rates)
df7<-data.frame(iterations=iteration,acceptance_probability=X_AM2_banana_th$acceptance_rates
df8<-data.frame(iterations=iteration,acceptance_probability=rep(0.234,n_iter+1))

ggplot(df1,aes(iterations,acceptance_probability))+geom_line(aes(color="MH"))+
      geom_line(data=df2,aes(color="AM"))+
      geom_line(data=df3,aes(color="AM2"))+
      geom_line(data=df4,aes(color="AM + shrinkage"))+
      geom_line(data=df5,aes(color="AM2 + shrinkage"))+
      geom_line(data=df6,aes(color="AM + thresholding"))+
      geom_line(data=df7,aes(color="AM2 + thresholding"))+
      geom_line(data=df8,aes(color="Optimal acceptance"))+
      labs(color="Alorithm:")
```




```
# all lines of the mean in the same plot with a legend
```

```
target=pi_norm_corr


X_MH = mcmc(target = target,
         n_iter = n_iter,
         x_1 = x_1,
         adapt=adapt)

## Running MCMC targeting  target with  200 iterations.
## Adaptation algorithm is:  AM .
## Covariance matrix estimator is:  Sample covariance .
## MCMC finished in 0.08550191 seconds.
## The last acceptance rate was: 0.28

X_AM = mcmc(target = target,
         n_iter = n_iter,
         x_1 = x_1,
         adapt=adapt,
         t_adapt = t_adapt,
         cov_estimator=cov_estimator
         )

## Running MCMC targeting  target with  200 iterations.
## Adaptation algorithm is:  AM .
## Covariance matrix estimator is:  Sample covariance .
## MCMC finished in 1.854948 seconds.
## The last acceptance rate was: 0.275

X_AM2 = mcmc(target = target,
         n_iter = n_iter,
         x_1 = x_1,
         adapt="AM2"
         )

## Running MCMC targeting  target with  200 iterations.
## Adaptation algorithm is:  AM2 .
## Covariance matrix estimator is:  Sample covariance .
## MCMC finished in 0.07970977 seconds.
## The last acceptance rate was: 0.28

X_AM_sh= mcmc(target = target,
         n_iter = n_iter,
         x_1 = x_1,
         adapt="AM",
         t_adapt = t_adapt,
         cov_estimator=cov_estimator1
         )
```

```
## Running MCMC targeting  target with  200 iterations.
## Adaptation algorithm is:  AM .
## Covariance matrix estimator is:  Shrinkage estimator .Estimating optimal shrinkage intens
##
##
## MCMC finished in 2.147528 seconds.
## The last acceptance rate was: 0.24
```

```
X_AM2_sh = mcmc(target = target,
         n_iter = n_iter,
         x_1 = x_1,
         adapt="AM2",
         cov_estimator=cov_estimator1
         )
```

```
## Running MCMC targeting  target with  200 iterations.
## Adaptation algorithm is:  AM2 .
## Covariance matrix estimator is:  Shrinkage estimator .
## MCMC finished in 0.07161546 seconds.
## The last acceptance rate was: 0.21
```

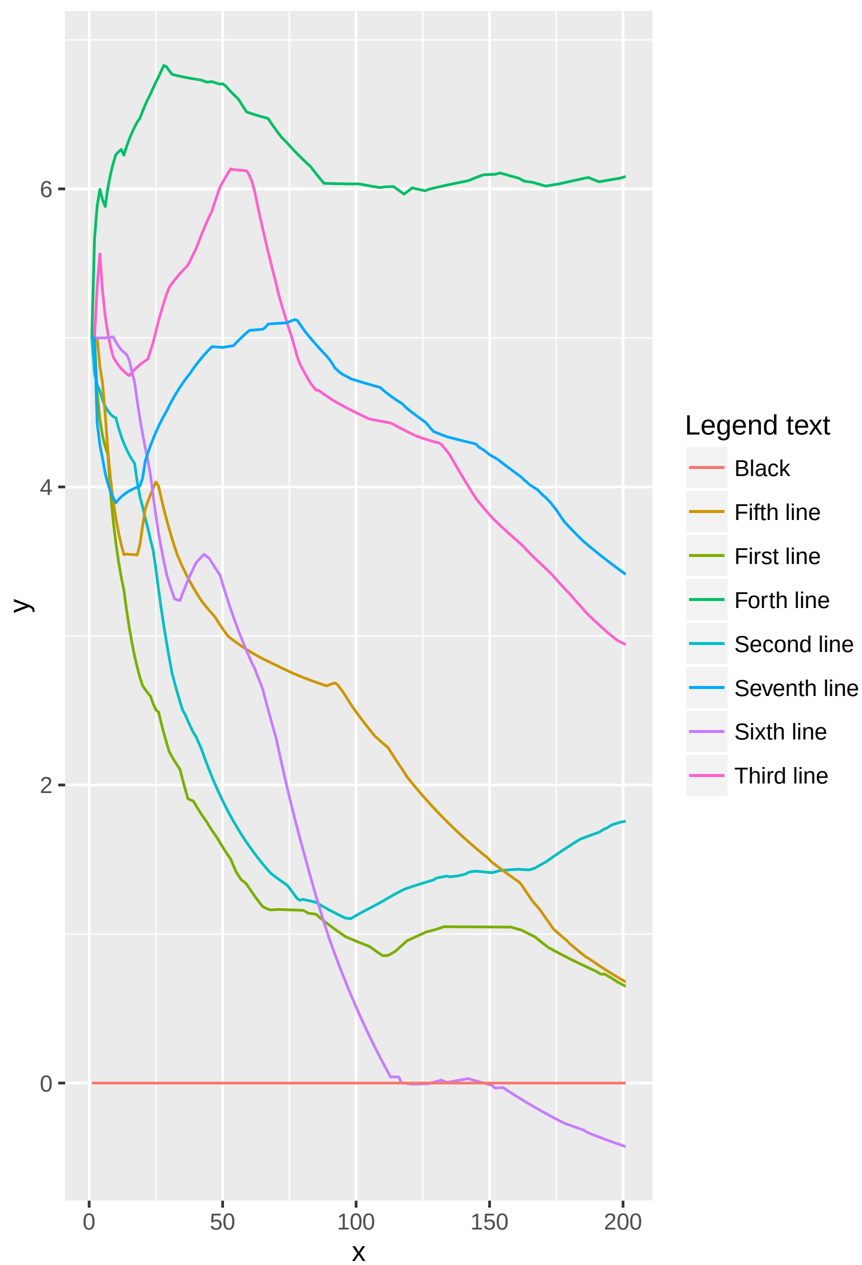
```
X_AM_th= mcmc(target = target,
         n_iter = n_iter,
         x_1 = x_1,
         adapt="AM",
         t_adapt = t_adapt,
         cov_estimator=cov_estimator2
         )
```

```
## Running MCMC targeting  target with  200 iterations.
## Adaptation algorithm is:  AM .
## Covariance matrix estimator is:  Thresholding estimator .
## MCMC finished in 0.2547455 seconds.
## The last acceptance rate was: 0.2
```

```
X_AM2_th = mcmc(target = target,
         n_iter = n_iter,
         x_1 = x_1,
         adapt="AM2",
         cov_estimator=cov_estimator2
         )
```

```
## Running MCMC targeting  target with  200 iterations.
## Adaptation algorithm is:  AM2 .
## Covariance matrix estimator is:  Thresholding estimator .
## MCMC finished in 0.07442594 seconds.
## The last acceptance rate was: 0.3
```

```r
df1<-data.frame(x=iteration,y=X_MH$sample_mean[,1])
df2<-data.frame(x=iteration,y=X_AM$sample_mean[,1])
df3<-data.frame(x=iteration,y=X_AM2$sample_mean[,1])
df4<-data.frame(x=iteration,y=X_AM_sh$sample_mean[,1])
df5<-data.frame(x=iteration,y=X_AM2_sh$sample_mean[,1])
df6<-data.frame(x=iteration,y=X_AM_th$sample_mean[,1])
df7<-data.frame(x=iteration,y=X_AM2_th$sample_mean[,1])
df8<-data.frame(x=iteration, y=rep(0,n_iter+1))

ggplot(df1,aes(x,y))+geom_line(aes(color="First line"))+
      geom_line(data=df2,aes(color="Second line"))+
      geom_line(data=df3,aes(color="Third line"))+
      geom_line(data=df4,aes(color="Forth line"))+
      geom_line(data=df5,aes(color="Fifth line"))+
      geom_line(data=df6,aes(color="Sixth line"))+
      geom_line(data=df7,aes(color="Seventh line"))+
      geom_line(data=df8,aes(color="Black"))+
      labs(color="Legend text")
```




```
# all lines of the mean in the same plot with a legend
```

3 A Bit About knitr

Whilst this demonstrates that the algorithms both approximately sample from the correct target distribution, there is no improvement in acceptance rate due to the adaptation steps. We require a less regular shaped target distribution to test whether adaptation improves our acceptance rate towards the optimal 0.234. For this we follow Haario et al in using a banana-shaped distribution. The following results show a significantly lower acceptance rate for the adaptive version of the algorithm.

The AM algorithm with banana target:

The MH algorithm with banana target:

We can see that the acceptance probability is closer to the optimal 0.234 with adaptation according to Haario et al.

4 Less naive covariance estimation

Naive empirical covariance estimators are unstable for high-dimensional problems with little data; the literature .

Following these two adaptive MH implementations, we are now looking to use something that is less naive than the vanilla estimator for the covariance matrix. In particular we have began testing the shrinkage and thresholding estimators as modifications to AM2. We will now test whether these estimators translate into better convergence by looking at their trajectories. We then plan to include burn in, and compare all algorithms in terms of the suboptimality factor following Roberts and Rosenthal (2009).

5 LaTeX

LaTeXitself is complicated if you've never used it before, but I'm sure you'll pick it up quickly: there are a lot of guides on the web. I recommend using the `align` environment (in the `amsmath` package) for displayed equations:

$$\begin{aligned} f(x) &= x^3 - x - 1 \\ g(y) &= y^4 + 2y \end{aligned}$$

You can cite in two ways using the `natbib` package: (Haario et al., 2001) and Haario et al. (2001).

References

A Gelman, GO Roberts, and WR Gilks. Efficient metropolis jumping rules. 1996.

Heikki Haario, Eero Saksman, and Johanna Tamminen. An adaptive metropolis algorithm. *Bernoulli*, 7(2):223–242, 04 2001. URL `http://projecteuclid.org/euclid.bj/1080222083`.

Gareth O. Roberts and Jeffrey S. Rosenthal. Examples of adaptive mcmc. *Journal of Computational and Graphical Statistics*, 18(2):349367, 2009. doi: 10.1198/jcgs.2009.06134. URL `http://dx.doi.org/10.1198/jcgs.2009.06134`.