

# The AdMit Package\*

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**Abstract:** This short note presents the R package **AdMit** which provides flexible functions to approximate a certain target distribution and to efficiently generate a sample of random draws from it, given only a kernel of the target density function. The estimation procedure is fully automatic and thus avoids the time-consuming and difficult task of tuning a sampling algorithm. To illustrate the use of the package, we apply the AdMit methodology to a bivariate bimodal distribution. We describe the use of the functions provided by the package and document the ability and relevance of the methodology to reproduce the shape of non-elliptical distributions.

*Keywords:* adaptive mixture, Student- $t$  distributions, importance sampling, independence chain Metropolis-Hastings algorithm, Bayesian inference, R software.

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# AdMit

**A package for constructing and using an adaptive mixture of Student- $t$  distributions as a flexible candidate distribution for efficient simulation.**

by David Ardia, Lennart F. Hoogerheide and Herman K. van Dijk

## Introduction

This note presents the package **AdMit** (Ardia et al., 2008, 2009), an R implementation of the adaptive mixture of Student- $t$  distributions (AdMit) procedure developed by Hoogerheide (2006); see also Hoogerheide et al. (2007); Hoogerheide and van Dijk (2008). The AdMit strategy consists of the construction of a mixture of Student- $t$  distributions which approximates a target distribution of interest. The fitting procedure relies only on a kernel of the target density, so that the normalizing constant is not required. In a second step, this approximation is used as an importance function in importance sampling or as a candidate density in the independence chain Metropolis-Hastings (M-H) algorithm to estimate characteristics of the target density. The estimation procedure is fully automatic and thus avoids the difficult task, especially for non-experts, of tuning a sampling algorithm. Typically, the target is a posterior distribution in a Bayesian analysis, where we indeed often only know a kernel of the posterior density.

In a *standard* case of importance sampling or the independence chain M-H algorithm, the candidate density is unimodal. If the target distribution is multimodal then some draws may have huge weights in the importance sampling approach and a second mode may be completely missed in the M-H strategy. As a consequence, the convergence behavior of these Monte Carlo integration methods is rather uncertain. Thus, an important problem is the choice of the importance or candidate density, especially when little is known a priori about the shape of the target density. For both importance sampling and the independence chain M-H, it holds that the candidate density should be *close* to the target density, and it is especially important that the tails of the candidate should not be thinner than those of the target.

Hoogerheide (2006) and Hoogerheide et al. (2007) mention several reasons why mixtures of Student- $t$  distributions are natural candidate densities. First, they can provide an accurate approximation to a wide variety of target densities, with substantial skewness and high kurtosis. Furthermore, they can deal with multi-modality and with non-elliptical shapes due to asymptotes. Second, this approximation can be constructed in a quick, iterative procedure and a mixture of Student- $t$  distributions is easy

to sample from. Third, the Student- $t$  distribution has fatter tails than the Normal distribution; especially if one specifies Student- $t$  distributions with few degrees of freedom, the risk is small that the tails of the candidate are thinner than those of the target distribution. Finally, Zeevi and Meir (1997) showed that under certain conditions any density function may be approximated to arbitrary accuracy by a convex combination of *basis* densities; the mixture of Student- $t$  distributions falls within their framework.

The package **AdMit** consists of three main functions: **AdMit**, **AdMitIS** and **AdMitMH**. The first one allows the user to fit a mixture of Student- $t$  distributions to a given density through its kernel function. The next two functions perform importance sampling and independence chain M-H sampling using the fitted mixture estimated by **AdMit** as the importance or candidate density, respectively.

To illustrate the use of the package, we apply the **AdMit** methodology to a bivariate bimodal distribution. We describe the use of the functions provided by the package and document the ability and relevance of the methodology to reproduce the shape of non-elliptical distributions.

## Illustration

This section presents the functions provided by the package **AdMit** with an illustration of a bivariate bimodal distribution. This distribution belongs to the class of conditionally Normal distributions proposed by Gelman and Meng (1991) with the property that the joint density is not Normal. It is not a posterior distribution, but it is chosen because it is a simple distribution with non-elliptical shapes so that it allows for an easy illustration of the **AdMit** approach.

Let  $X_1$  and  $X_2$  be two random variables, for which  $X_1$  is Normally distributed given  $X_2$  and vice versa. Then, the joint distribution, after location and scale transformations in each variable, can be written as (see Gelman and Meng, 1991):

$$p(\mathbf{x}) \propto k(\mathbf{x}) \doteq \exp \left[ -\frac{1}{2}(Ax_1^2x_2^2 + x_1^2 + x_2^2 - 2Bx_1x_2 - 2C_1x_1 - 2C_2x_2) \right] \quad (1)$$

where  $p(\mathbf{x})$  denotes a density,  $k(\mathbf{x})$  a kernel and  $\mathbf{x} \doteq (x_1, x_2)'$  for notational purposes.  $A, B, C_1$  and  $C_2$  are constants; we consider an asymmetric case in which  $A = 5, B = 5, C_1 = 3, C_2 = 3.5$  in what follows.

The adaptive mixture approach determines the number of mixture components  $H$ , the mixing probabilities, the modes and scale matrices of the components in such a way that the mixture density  $q(\mathbf{x})$  approximates the target density  $p(\mathbf{x})$  of which we only know a kernel function  $k(\mathbf{x})$  with  $\mathbf{x} \in \mathbb{R}^d$ . Typically,

$k(\mathbf{x})$  will be a posterior density kernel for a vector of model parameters  $\mathbf{x}$ .

The AdMit strategy consists of the following steps:

- (0) Initialization: computation of the mode and scale matrix of the first component, and drawing a sample from this Student- $t$  distribution;
- (1) Iterate on the number of components: add a new component that covers a part of the space of  $\mathbf{x}$  where the previous mixture density was relatively small, as compared to  $k(\mathbf{x})$ ;
- (2) Optimization of the mixing probabilities;
- (3) Drawing a sample  $\{\mathbf{x}^{[i]}\}$  from the new mixture  $q(\mathbf{x})$ ;
- (4) Evaluation of importance sampling weights  $\{k(\mathbf{x}^{[i]})/q(\mathbf{x}^{[i]})\}$ . If the coefficient of variation, i.e. the standard deviation divided by the mean, of the weights has converged, then stop. Otherwise, go to step (1). By default, the adaptive procedure stops if the relative change in the coefficient of variation of the importance sampling weights caused by adding one new Student- $t$  component to the candidate mixture is less than 10%.

There are two main reasons for using the coefficient of variation of the importance sampling weights as a measure of the fitting quality. First, it is a natural, intuitive measure of quality of the candidate as an approximation to the target. If the candidate and the target distributions coincide, all importance sampling weights are equal, so that the coefficient of variation is zero. For a poor candidate that not even roughly approximates the target, some importance sampling weights are huge while most are (almost) zero, so that the coefficient of variation is high. The better the candidate approximates the target, the more evenly the weight is divided among the candidate draws, and the smaller the coefficient of variation of the importance sampling weights. Second, Geweke (1989) argues that a reasonable objective in the choice of an importance density is the minimization of the variance, or equivalently the coefficient of variation, of the importance weights. We prefer to quote the coefficient of variation because it does not depend on the number of draws or the integration constant of the posterior density kernel, unlike the standard deviation of the scaled or unscaled importance weights, respectively. The coefficient of variation merely reflects the quality of the candidate as an approximation to the target.

Note also that all Student- $t$  components in the mixture approximation  $q(\mathbf{x})$  have the same degrees of freedom parameter. Moreover, this value is not determined by the procedure but set by the user; by default, the algorithm uses the value one (i.e. the approximation density is a mixture of Cauchy) since i)

it enables the method to deal with fat-tailed target distributions and ii) it makes it easier for the iterative procedure to detect modes that are far apart. There may be a trade-off between efficiency and robustness at this point: setting the degrees of freedom to one reflects that we find a higher robustness more valuable than a slight possible gain in efficiency.

The core function provided by the package is the function `AdMit`. The main arguments of the function are: `KERNEL`, a kernel function of the target density on which the approximation is constructed. This function must contain the logical argument `log`. When `log = TRUE`, the function `KERNEL` returns the logarithm value of the kernel function; this is used for numerical stability. `mu0` is the starting value of the first stage optimization; it is a vector whose length corresponds to the length of the first argument in `KERNEL`. `Sigma0` is the (symmetric positive definite) scale matrix of the first component. If a matrix is provided by the user, it is used as the scale matrix of the first component and then `mu0` is used as the mode of the first component (instead of a starting value for optimization). `control` is a list of tuning parameters, containing in particular: `df` (default: 1), the degrees of freedom of the mixture components and `CVtol` (default: 0.1), the tolerance of the relative change of the coefficient of variation. For further details, the reader is referred to the documentation manual (by typing `?AdMit`) or to Ardia et al. (2009). Finally, the last argument of `AdMit` is `...` which allows the user to pass additional arguments to the function `KERNEL`.

Let us come back to our bivariate conditionally Normal distribution. First, we need to code the kernel:

```
> GelmanMeng <- function(x, log = TRUE)
+ {
+   if (is.vector(x))
+     x <- matrix(x, nrow = 1)
+   r <- -0.5 * ( 5 * x[,1]^2 * x[,2]^2
+               + x[,1]^2 + x[,2]^2
+               - 10 * x[,1] * x[,2]
+               - 6 * x[,1] - 7 * x[,2] )
+   if (!log)
+     r <- exp(r)
+   as.vector(r)
+ }
```

Note that the argument `log` is set to `TRUE` by default so that the function outputs the logarithm of the kernel. Moreover, the function is vectorized to speed up the computations. The contour plot of `GelmanMeng` is displayed in the left part of Figure 1.

We now use the function `AdMit` to find a suitable approximation for the density whose kernel is `GelmanMeng`. We use the starting value `mu0 = c(0, 0.1)` for the first stage optimization and assign the result of the function to `outAdMit`.

```
> set.seed(1234)
> outAdMit <- AdMit(KERNEL = GelmanMeng,
+                  mu0 = c(0, 0.1))
```

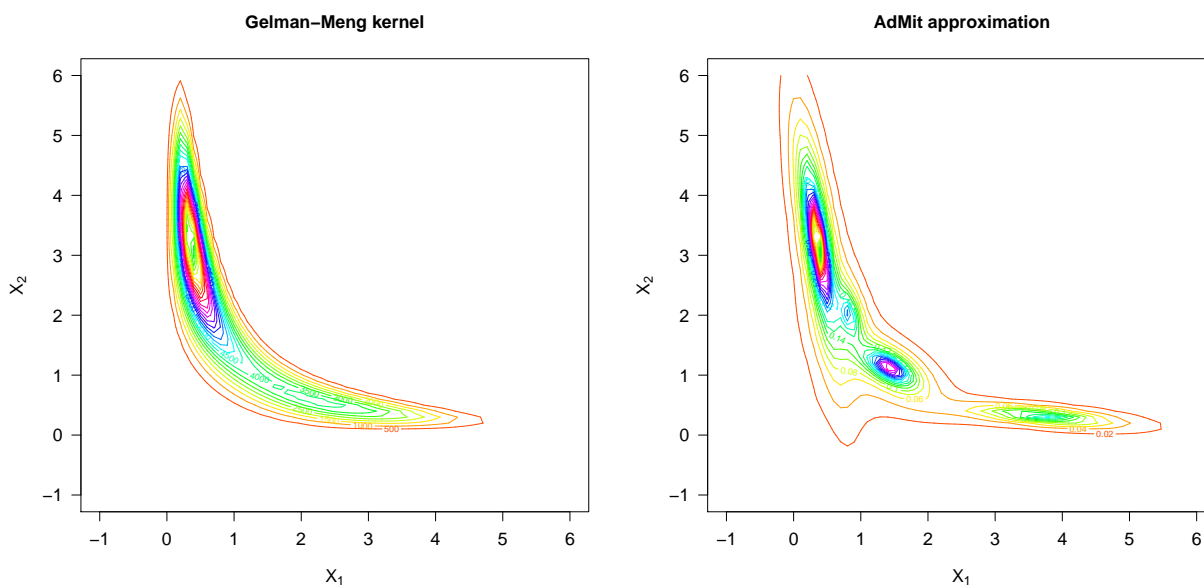


Figure 1: Left: contour plot of the kernel `GelmanMeng`. Right: contour plot of the four-component Student- $t$  mixture approximation estimated by the function `AdMit`.

```

$CV
[1] 8.0737 1.7480 0.9557 0.8807

$mit
$mit$p
  cmp1    cmp2    cmp3    cmp4
0.54707 0.14268 0.21053 0.09972

$mit$mu
      k1    k2
cmp1 0.3640 3.2002
cmp2 3.7088 0.3175
cmp3 1.4304 1.1240
cmp4 0.8253 2.0261

$mit$Sigma
      k1k1    k1k2    k2k1    k2k2
cmp1 0.03903 -0.15606 -0.15606 1.22561
cmp2 0.86080 -0.08398 -0.08398 0.02252
cmp3 0.13525 -0.06743 -0.06743 0.09520
cmp4 0.03532 -0.04072 -0.04072 0.21735

$mit$df
[1] 1

$summary
  H METHOD.mu TIME.mu METHOD.p TIME.p    CV
1 1  BFGS    0.21    NONE    0.00 8.0737
2 2  BFGS    0.08  NLMINB    0.08 1.7480
3 3  BFGS    0.12  NLMINB    0.08 0.9557
4 4  BFGS    0.20  NLMINB    0.19 0.8807

```

The output of the function `AdMit` is a list. The first component is `CV`, a vector of length  $H$  which gives the value of the coefficient of variation of the importance sampling weights at each step of the adaptive fitting procedure. The second component is `mit`, a list

which consists of four components giving information on the fitted mixture of Student- $t$  distributions: `p` is a vector of length  $H$  of mixing probabilities, `mu` is a  $H \times d$  matrix whose rows give the modes of the mixture components, `Sigma` is a  $H \times d^2$  matrix whose rows give the scale matrices (in vector form) of the mixture components and `df` is the degrees of freedom of the Student- $t$  components. The third component of the list returned by `AdMit` is `summary`. This is a data frame containing information on the adaptive fitting procedure. We refer the reader to the documentation manual for further details.

For the kernel `GelmanMeng`, the approximation constructs a mixture of four components. The value of the coefficient of variation decreases from 8.0737 to 0.8807. A contour plot of the four-component approximation is displayed in the right-hand side of Figure 1. This graph is produced using the function `dMit` which returns the density of the mixture given by the output `outAdMit$mit`. The contour plot illustrates that the four-component mixture provides a good approximation of the density: the areas with substantial target density mass are covered by sufficient density mass of the mixture approximation.

Once the adaptive mixture of Student- $t$  distributions is fitted to the density using a kernel, the approximation provided by `AdMit` is used as the importance sampling density in importance sampling or as the candidate density in the independence chain M-H algorithm.

The `AdMit` package contains the `AdMitIS` function which performs importance sampling using the mixture approximation in `outAdMit$mit` as the importance density. The arguments of the function `AdMitIS` are: (i)  $N$ , the number of draws used in im-

portance sampling; (ii) `KERNEL`, a kernel function of the target density; (iii) `G`, the function of which the expectation  $\mathbb{E}_p[g(\mathbf{x})]$  is estimated; By default, the function `G` is the identity so that the function outputs a vector containing the mean estimates for the components of  $\mathbf{x}$ . Alternative functions may be provided by the user to obtain other quantities of interest for  $p(\mathbf{x})$ . The only requirement is that the function outputs a matrix; (iv) `mit`, a list providing information on the mixture approximation; (v) `...` allows additional parameters to be passed to the function `KERNEL` and/or `G`.

Let us apply the function `AdMitIS` to the kernel `GelmanMeng` using the approximation `outAdMit$mit`:

```
> outAdMitIS <- AdMitIS(N = 1e5,
+                       KERNEL = GelmanMeng,
+                       mit = outAdMit$mit)

$ghat
[1] 0.9556 2.2465

$NSE
[1] 0.003833 0.005639

$RNE
[1] 0.6038 0.5536
```

The output of the function `AdMitIS` is a list. The first component is `ghat`, the importance sampling estimator of  $\mathbb{E}_p[g(\mathbf{x})]$ . The second component is `NSE`, a vector containing the numerical standard errors (the variation of the estimates that can be expected if the simulations were to be repeated) of the components of `ghat`. The third component is `RNE`, a vector containing the relative numerical efficiencies of the components of `ghat` (the ratio between an estimate of the variance of an estimator based on direct sampling and the importance sampling estimator's estimated variance with the same number of draws). `RNE` is an indicator of the efficiency of the chosen importance function; if target and importance densities coincide, `RNE` equals one, whereas a very poor importance density will have a `RNE` close to zero. Both `NSE` and `RNE` are estimated by the method given in Geweke (1989).

Further, the `AdMit` package contains the `AdMitMH` function which uses the mixture approximation in `outAdMit$mit` as the candidate density in the independence chain M-H algorithm. The arguments of the function `AdMitMH` are: (i) `N`, the length of the MCMC sequence of draws; (ii) `KERNEL`, a kernel function of the target density; (iii) `mit`, a list providing information on the mixture approximation; (iv) `...` allows additional parameters to be passed to the function `KERNEL`.

Let us apply the function `AdMitMH` to the kernel `GelmanMeng` using the approximation `outAdMit$mit`:

```
> outAdMitMH <- AdMitMH(N = 101000,
+                       KERNEL = GelmanMeng,
+                       mit = outAdMit$mit)
```

```
$draws
      k1      k2
1  7.429e-01 3.021e-01
2  7.429e-01 3.021e-01
3  7.429e-01 3.021e-01
4  1.352e+00 1.316e+00
5  1.011e+00 1.709e+00
6  1.011e+00 1.709e+00
7  1.005e+00 1.386e+00
...

$accept
[1] 0.5119
```

The output of the function `AdMitMH` is a list of two components. The first component is `draws`, a  $N \times d$  matrix containing draws from the target density  $p(\mathbf{x})$  in its rows. The second component is `accept`, the acceptance rate of the independence chain M-H algorithm.

The package `coda` (Plummer et al., 2008) can be used to check the convergence of the MCMC chain and obtain quantities of interest for  $p(\mathbf{x})$ . Here, for simplicity, we discard the first 1'000 draws as a burn-in sample and transform the output `outAdMitMH$draws` in a `mcmc` object using the function `as.mcmc` provided by `coda`. A summary of the MCMC chain can be obtained using `summary`:

```
> library("coda")
> draws <- as.mcmc(outAdMitMH$draws)
> window(draws, start = 1001)
> colnames(draws) <- c("X1", "X2")
> summary(draws)$stat

      Mean      SD Naive SE Time-series SE
X1 0.9643 0.9476 0.002996      0.004327
X2 2.2388 1.3284 0.004201      0.006232
```

We note that the mean estimates are close to the values obtained with the function `AdMitIS`. The relative numerical efficiency (`RNE`) can be computed using the functions `effectiveSize` and `niter`:

```
> effectiveSize(draws) / niter(draws)

      X1      X2
0.3082 0.3055
```

These relative numerical efficiencies reflect the good quality of the candidate density in the independence chain M-H algorithm.

The approach is compared to the standard Gibbs sampler, which is extremely easy to implement here since the full conditional densities are Normals. We generated  $N = 101000$  draws from a Gibbs sampler using the first 1'000 draws as a burn-in period. In this case, the `RNE` were 0.06411 and 0.07132, respectively. In Figure 2 we display the autocorrelogram for the MCMC output of the `AdMitMH` function (upper graphs) together with the autocorrelogram of the Gibbs (lower part). We clearly notice that the Gibbs sequence is mixing much more slowly, explaining the

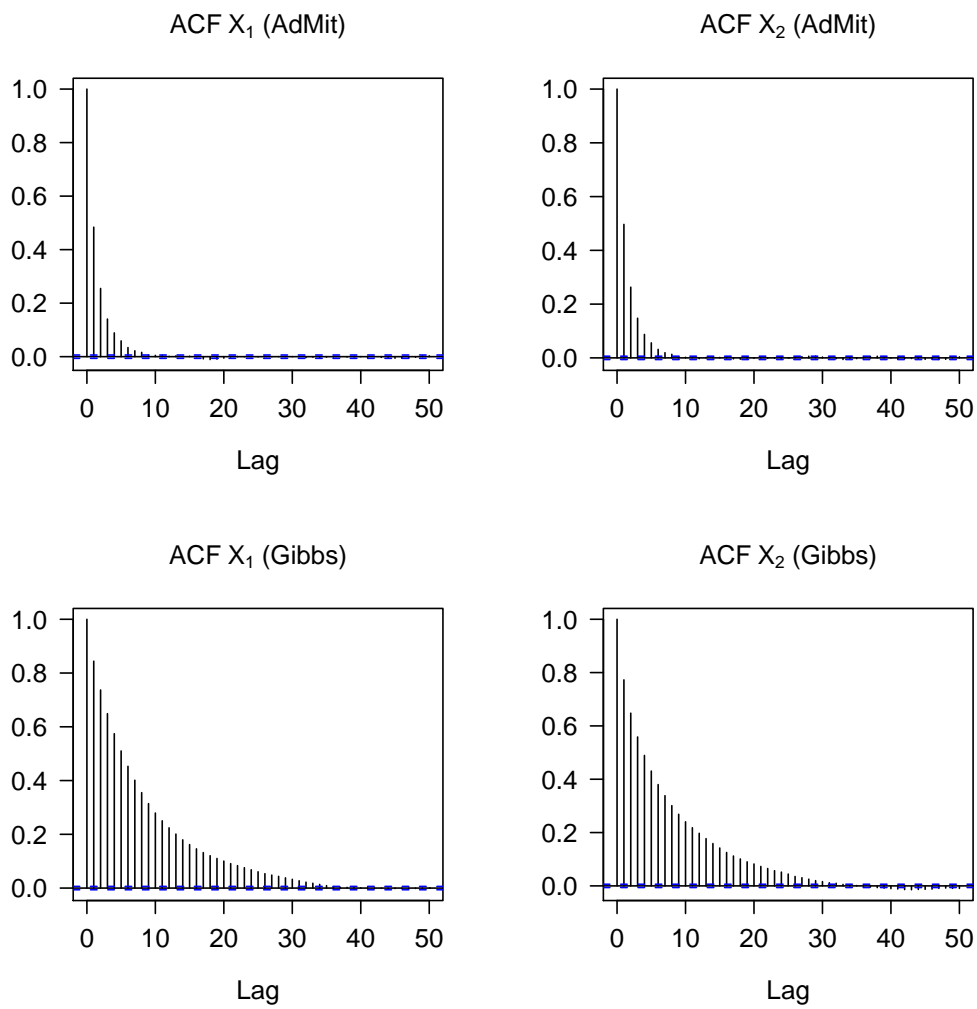


Figure 2: Upper graphs: Autocorrelation function (ACF) for the AdMitMH output. Lower graphs: ACF for the Gibbs output.

lower RNE values. This example illustrates the phenomenon that the autocorrelation in the Gibbs sequence may be high when assessing a non-elliptical distribution, and that the AdMit approach may overcome this.

## Summary

This note presented the package **AdMit** which provides functions to approximate and sample from a certain target distribution given only a kernel of the target density function. The estimation procedure is fully automatic and thus avoids the time-consuming and difficult task of tuning a sampling algorithm. The use of the package has been illustrated in a bivariate bimodal distribution.

Interested users are referred to Ardia et al. (2009) for a more complete discussion on the **AdMit** package. The article provides a more extensive introduction of the package usage as well as an illustration of the relevance of the AdMit procedure with the Bayesian estimation of a mixture of ARCH model fitted to foreign exchange log-returns data. The methodology is compared to standard cases of importance sampling and the Metropolis-Hastings algorithm using a naive candidate and with the Griddy-Gibbs approach. It is shown that for investigating means and particularly tails of the joint posterior distribution the AdMit approach is preferable.

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