# Package 'mvnfast'

October 10, 2016

**Type** Package

**Title** Fast Multivariate Normal and Student's t Methods

**Version** 0.1.7

**Date** 2016-10-10

**Author** Matteo Fasiolo, using the C++ parallel RNG of Thijs van den Berg and Ziggurat algorithm of Jens Maurer and Steven Watanabe (boost)

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**Description** Provides computationally efficient tools related to the multivariate normal and Student's t distributions. The main functionalities are: simulating multivariate random vectors, evaluating multivariate normal or Student's t densities and Mahalanobis distances. These tools are very efficient thanks to the use of C++ code and of the OpenMP API.

**License** GPL (>= 2.0)

**URL** https://github.com/mfasiolo/mvnfast, www.sitmo.com

**Imports** Rcpp (>= 0.10.4)

**Suggests** knitr, testthat, mvtnorm, microbenchmark, MASS, plyr, RhpcBLASctl

**LinkingTo** Rcpp, RcppArmadillo, BH

**VignetteBuilder** knitr

**RoxygenNote** 5.0.1

**NeedsCompilation** yes

**Repository** CRAN

**Date/Publication** 2016-10-10 13:51:57

## R topics documented:

dmvn *Fast computation of the multivariate normal density.*

## Description

Fast computation of the multivariate normal density.

## Usage

```
dmvn(X, mu, sigma, log = FALSE, ncores = 1, isChol = FALSE)
```

## Arguments

| | |
|---|---|
| X | matrix n by d where each row is a d dimensional random vector. Alternatively X can be a d-dimensional vector. |
| mu | vector of length d, representing the mean of the distribution. |
| sigma | covariance matrix (d x d). Alternatively it can be the cholesky decomposition of the covariance. In that case isChol should be set to TRUE. |
| log | boolean set to true the logarithm of the pdf is required. |
| ncores | Number of cores used. The parallelization will take place only if OpenMP is supported. |
| isChol | boolean set to true is sigma is the cholesky decomposition of the covariance matrix. |

## Value

A vector of length n where the i-the entry contains the pdf of the i-th random vector.

## Author(s)

Matteo Fasiolo <matteo.fasiolo@gmail.com>

## Examples

```
N <- 100
d <- 5
mu <- 1:d
X <- t(t(matrix(rnorm(N*d), N, d)) + mu)
tmp <- matrix(rnorm(d^2), d, d)
mcov <- tcrossprod(tmp, tmp)  + diag(0.5, d)
myChol <- chol(mcov)

head(dmvn(X, mu, mcov), 10)
head(dmvn(X, mu, myChol, isChol = TRUE), 10)

## Not run:
```

```
# Performance comparison
library(mvtnorm)
library(microbenchmark)

a <- cbind(
      dmvn(X, mu, mcov),
      dmvn(X, mu, myChol, isChol = TRUE),
      dmvnorm(X, mu, mcov))

# Check if we get the same output as dmvnorm()
a[ , 1] / a[, 3]
a[ , 2] / a[, 3]

microbenchmark(dmvn(X, mu, myChol, isChol = TRUE),
               dmvn(X, mu, mcov),
               dmvnorm(X, mu, mcov))

detach("package:mvtnorm", unload=TRUE)

## End(Not run)
```

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dmvt *Fast computation of the multivariate Student's t density.*

---

## Description

Fast computation of the multivariate Student's t density.

## Usage

```
dmvt(X, mu, sigma, df, log = FALSE, ncores = 1, isChol = FALSE)
```

## Arguments

| | |
|---|---|
| X | matrix n by d where each row is a d dimensional random vector. Alternatively X can be a d-dimensional vector. |
| mu | vector of length d, representing the mean of the distribution. |
| sigma | scale matrix (d x d). Alternatively it can be the cholesky decomposition of the scale matrix. In that case isChol should be set to TRUE. Notice that ff the degrees of freedom (the argument df) is larger than 2, the Cov(X)=sigma*df/(df-2). |
| df | a positive scalar representing the degrees of freedom. |
| log | boolean set to true the logarithm of the pdf is required. |
| ncores | Number of cores used. The parallelization will take place only if OpenMP is supported. |
| isChol | boolean set to true is sigma is the cholesky decomposition of the covariance matrix. |

## Details

There are in fact many candidates for the multivariate generalization of Student's t-distribution, here we use the parametrization described here https://en.wikipedia.org/wiki/Multivariate_t-distribution. NB: at the moment the parallelization does not work properly on Solaris OS when ncores>1. Hence, dmvt() checks if the OS is Solaris and, if this the case, it imposes ncores==1.

## Value

A vector of length n where the i-the entry contains the pdf of the i-th random vector.

## Author(s)

Matteo Fasiolo <matteo.fasiolo@gmail.com>

## Examples

```
N <- 100
d <- 5
mu <- 1:d
df <- 4
X <- t(t(matrix(rnorm(N*d), N, d)) + mu)
tmp <- matrix(rnorm(d^2), d, d)
mcov <- tcrossprod(tmp, tmp)  + diag(0.5, d)
myChol <- chol(mcov)

head(dmvt(X, mu, mcov, df = df), 10)
head(dmvt(X, mu, myChol, df = df, isChol = TRUE), 10)
```

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maha *Fast computation of squared mahalanobis distance between all rows of* X *and the vector* mu *with respect to sigma.*

---

## Description

Fast computation of squared mahalanobis distance between all rows of X and the vector mu with respect to sigma.

## Usage

```
maha(X, mu, sigma, ncores = 1, isChol = FALSE)
```

## Arguments

| | |
|---|---|
| X | matrix n by d where each row is a d dimensional random vector. Alternatively X can be a d-dimensional vector. |
| mu | vector of length d, representing the central position. |
| sigma | covariance matrix (d x d). Alternatively is can be the cholesky decomposition of the covariance. In that case isChol should be set to TRUE. |
| ncores | Number of cores used. The parallelization will take place only if OpenMP is supported. |
| isChol | boolean set to true is sigma is the cholesky decomposition of the covariance matrix. |

## Value

a vector of length n where the i-the entry contains the square mahalanobis distance i-th random vector.

## Author(s)

Matteo Fasiolo <matteo.fasiolo@gmail.com>

## Examples

```
N <- 100
d <- 5
mu <- 1:d
X <- t(t(matrix(rnorm(N*d), N, d)) + mu)
tmp <- matrix(rnorm(d^2), d, d)
mcov <- tcrossprod(tmp, tmp)
myChol <- chol(mcov)

rbind(head(maha(X, mu, mcov), 10),
      head(maha(X, mu, myChol, isChol = TRUE), 10),
      head(mahalanobis(X, mu, mcov), 10))

## Not run:
# Performance comparison
library(microbenchmark)

a <- cbind(
  maha(X, mu, mcov),
  maha(X, mu, myChol, isChol = TRUE),
  mahalanobis(X, mu, mcov))

# Same output as mahalanobis
a[ , 1] / a[, 3]
a[ , 2] / a[, 3]

microbenchmark(maha(X, mu, mcov),
               maha(X, mu, myChol, isChol = TRUE),
               mahalanobis(X, mu, mcov))
```

```
## End(Not run)
```

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ms *Mean-shift mode seeking algorithm*

---

## Description

Given a sample from a d-dimensional distribution, an initialization point and a bandwidth the algorithm finds the nearest mode of the corresponding Gaussian kernel density.

## Usage

```
ms(X, init, H, tol = 1e-06, ncores = 1, store = FALSE)
```

## Arguments

| | |
|---|---|
| X | n by d matrix containing the data. |
| init | d-dimensional vector containing the initial point for the optimization. By default it is equal to `colMeans(X)`. |
| H | Positive definite bandwidth matrix representing the covariance of each component of the Gaussian kernel density. |
| tol | Tolerance used to assess the convergence of the algorithm, which is stopped if the absolute values of increments along all the dimensions are smaller then tol at any iteration. Default value is 1e-6. |
| ncores | Number of cores used. The parallelization will take place only if OpenMP is supported. |
| store | If `FALSE` only the latest iteration is returned, if `TRUE` the function will return a matrix where the i-th row is the position of the algorithms at the i-th iteration. |

## Value

A list where `estim` is a d-dimensional vector containing the last position of the algorithm, while `traj` is a matrix with d-colums representing the trajectory of the algorithm along each dimension. If `store == FALSE` the whole trajectory is not stored and `traj = NULL`.

## Author(s)

Matteo Fasiolo <matteo.fasiolo@gmail.com>.

## Examples

```
set.seed(434)

# Simulating multivariate normal data
N <- 1000
mu <- c(1, 2)
sigma <- matrix(c(1, 0.5, 0.5, 1), 2, 2)
X <- rmvn(N, mu = mu, sigma = sigma)

# Plotting the true density function
steps <- 100
range1 <- seq(min(X[ , 1]), max(X[ , 1]), length.out = steps)
range2 <- seq(min(X[ , 2]), max(X[ , 2]), length.out = steps)
grid <- expand.grid(range1, range2)
vals <- dmvn(as.matrix(grid), mu, sigma)

contour(z = matrix(vals, steps, steps),  x = range1, y = range2, xlab = "X1", ylab = "X2")
points(X[ , 1], X[ , 2], pch = '.')

# Estimating the mode from "nrep" starting points
nrep <- 10
index <- sample(1:N, nrep)
for(ii in 1:nrep) {
  start <- X[index[ii], ]
  out <- ms(X, init = start, H = 0.1 * sigma, store = TRUE)
  lines(out$traj[ , 1], out$traj[ , 2], col = 2, lwd = 2)
  points(out$final[1], out$final[2], col = 4, pch = 3, lwd = 3) # Estimated mode (blue)
  points(start[1], start[2], col = 2, pch = 3, lwd = 3)         # ii-th starting value
}
```

---

`rmvn` *Fast simulation of multivariate normal random variables*

---

## Description

Fast simulation of multivariate normal random variables

## Usage

```
rmvn(n, mu, sigma, ncores = 1, isChol = FALSE, A = NULL)
```

## Arguments

| | |
|---|---|
| `n` | number of random vectors to be simulated. |
| `mu` | vector of length d, representing the mean. |
| `sigma` | covariance matrix (d x d). Alternatively is can be the cholesky decomposition of the covariance. In that case `isChol` should be set to `TRUE`. |

| | |
|---|---|
| ncores | Number of cores used. The parallelization will take place only if OpenMP is supported. |
| isChol | boolean set to true is sigma is the cholesky decomposition of the covariance matrix. |
| A | an (optional) numeric matrix of dimension (n x d), which will be used to store the output random variables. It is useful when n and d are large and one wants to call rmvn() several times, without reallocating memory for the whole matrix each time. NB: the element of A must be of class "numeric". |

## Details

Notice that this function does not use one of the Random Number Generators (RNGs) provided by R, but one of the parallel cryptographic RNGs described in (Salmon et al., 2011). It is important to point out that this RNG can safely be used in parallel, without risk of collisions between parallel sequence of random numbers. The initialization of the RNG depends on R's seed, hence the set.seed() function can be used to obtain reproducible results. Notice though that changing ncores causes most of the generated numbers to be different even if R's seed is the same (see example below). NB: at the moment the RNG does not work properly on Solaris OS when ncores>1. Hence, rmvn() checks if the OS is Solaris and, if this the case, it imposes ncores==1.

## Value

If A==NULL (default) the output is an (n x d) matrix where the i-th row is the i-th simulated vector. If A!=NULL then the random vector are store in A, which is provided by the user, and the function returns NULL.

## Author(s)

Matteo Fasiolo <matteo.fasiolo@gmail.com>, C++ RNG engine by Thijs van den Berg <http://sitmo.com/>.

## References

John K. Salmon, Mark A. Moraes, Ron O. Dror, and David E. Shaw (2011). Parallel Random Numbers: As Easy as 1, 2, 3. D. E. Shaw Research, New York, NY 10036, USA.

## Examples

```
d <- 5
mu <- 1:d

# Creating covariance matrix
tmp <- matrix(rnorm(d^2), d, d)
mcov <- tcrossprod(tmp, tmp)

set.seed(414)
rmvn(4, 1:d, mcov)

set.seed(414)
rmvn(4, 1:d, mcov)
```

```
set.seed(414)
rmvn(4, 1:d, mcov, ncores = 2) # r.v. generated on the second core are different

###### Here we create the matrix that will hold the simulated random variables upfront.
A <- matrix(NA, 4, d)
class(A) <- "numeric" # This is important. We need the elements of A to be of class "numeric".

set.seed(414)
rmvn(4, 1:d, mcov, ncores = 2, A = A) # This returns NULL ...
A                                     # ... but the result is here
```

---

`rmvt` *Fast simulation of multivariate Student's t random variables*

---

## Description

Fast simulation of multivariate Student's t random variables

## Usage

```
rmvt(n, mu, sigma, df, ncores = 1, isChol = FALSE, A = NULL)
```

## Arguments

| | |
|---|---|
| `n` | number of random vectors to be simulated. |
| `mu` | vector of length d, representing the mean of the distribution. |
| `sigma` | scale matrix (d x d). Alternatively it can be the cholesky decomposition of the scale matrix. In that case isChol should be set to TRUE. Notice that ff the degrees of freedom (the argument `df`) is larger than 2, the `Cov(X)=sigma*df/(df-2)`. |
| `df` | a positive scalar representing the degrees of freedom. |
| `ncores` | Number of cores used. The parallelization will take place only if OpenMP is supported. |
| `isChol` | boolean set to true is `sigma` is the cholesky decomposition of the covariance matrix. |
| `A` | an (optional) numeric matrix of dimension (n x d), which will be used to store the output random variables. It is useful when n and d are large and one wants to call `rmvn()` several times, without reallocating memory for the whole matrix each time. NB: the element of `A` must be of class "numeric". |

## Details

There are in fact many candidates for the multivariate generalization of Student's t-distribution, here we use the parametrization described here https://en.wikipedia.org/wiki/Multivariate_t-distribution.

Notice that rmvt() does not use one of the Random Number Generators (RNGs) provided by R, but one of the parallel cryptographic RNGs described in (Salmon et al., 2011). It is important to point out that this RNG can safely be used in parallel, without risk of collisions between parallel sequence of random numbers. The initialization of the RNG depends on R's seed, hence the set.seed() function can be used to obtain reproducible results. Notice though that changing ncores causes most of the generated numbers to be different even if R's seed is the same (see example below). NB: at the moment the RNG does not work properly on Solaris OS when ncores>1. Hence, rmvt() checks if the OS is Solaris and, if this the case, it imposes ncores==1.

## Value

If A==NULL (default) the output is an (n x d) matrix where the i-th row is the i-th simulated vector. If A!=NULL then the random vector are store in A, which is provided by the user, and the function returns NULL.

## Author(s)

Matteo Fasiolo <matteo.fasiolo@gmail.com>, C++ RNG engine by Thijs van den Berg <http://sitmo.com/>.

## References

John K. Salmon, Mark A. Moraes, Ron O. Dror, and David E. Shaw (2011). Parallel Random Numbers: As Easy as 1, 2, 3. D. E. Shaw Research, New York, NY 10036, USA.

## Examples

```
d <- 5
mu <- 1:d
df <- 4

# Creating covariance matrix
tmp <- matrix(rnorm(d^2), d, d)
mcov <- tcrossprod(tmp, tmp) + diag(0.5, d)

set.seed(414)
rmvt(4, 1:d, mcov, df = df)

set.seed(414)
rmvt(4, 1:d, mcov, df = df)

set.seed(414)
rmvt(4, 1:d, mcov, df = df, ncores = 2) # These will not match the r.v. generated on a single core.

###### Here we create the matrix that will hold the simulated random variables upfront.
A <- matrix(NA, 4, d)
class(A) <- "numeric" # This is important. We need the elements of A to be of class "numeric".

set.seed(414)
rmvt(4, 1:d, mcov, df = df, ncores = 2, A = A) # This returns NULL ...
A                                     # ... but the result is here
```

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