mvtnorm: New Numerical Algorithm for Multivariate Normal Probabilities

by Xuefei Mi, Tetsuhisa Miwa and Torsten Hothorn

Miwa et al. (2003) proposed a numerical algorithm for evaluating multivariate normal probabilities. Starting with version 0.9-0 of the **mvtnorm** package (Hothorn et al., 2001; Genz et al., 2008), this algorithm is available to the R community. We give a brief introduction to Miwa's procedure and compare it, with respect to computing time and accuracy, to a quasi-randomized Monte-Carlo procedure proposed by Genz and Bretz (1999), which has been available through **mvtnorm** for some years now.

The new algorithm is applicable to problems with dimension smaller than 20, whereas the procedures by Genz and Bretz (1999) can be used to evaluate 1000-dimensional normal distributions. At the end of this article, a suggestion is given for choosing a suitable algorithm in different situations.

Introduction

An algorithm for calculating any non-centered orthant probability of a non-singular multivariate normal distribution is described by Miwa et al. (2003). The probability function in a one-sided problem is

$$\begin{aligned} P_m(\mu, \mathbf{R}) &= \mathbb{P}\{X_i \geq 0; 1 \leq i \leq m\} \\ &= \int_0^\infty \dots \int_0^\infty \phi_m(\mathbf{x}; \mu, \mathbf{R})\, dx_1 \dots dx_m \end{aligned}$$

where $\mu = (\mu_1, ..., \mu_m)^\top$ is the mean and and $\mathbf{R} = (\rho_{ij})$ the correlation matrix of m multivariate normal distributed random variables $X_1, \dots, X_m \sim \mathcal{N}_m(\mu, \mathbf{R})$. The function ϕ_m denotes the density function of the m-dimensional normal distribution with mean μ and correlation matrix $\mathbf{R}$.

The distribution function for $\mathbf{c} = (c_1, \dots, c_m)$ can be expressed as:

$$\begin{aligned} F_m(\mathbf{c}) &= \mathbb{P}\{X_i \leq c_i; 1 \leq i \leq m\} \\ &= \mathbb{P}\{-X_i \geq -c_i; 1 \leq i \leq m\} \\ &= P_m(-\mu + \mathbf{c}, \mathbf{R}). \end{aligned}$$

The m-dimensional non-centered orthant one-sided probability can be calculated from at most $(m-1)!$ non-centered probabilities with positive definite tridiagonal correlation matrix. The algorithm for calculating such probabilities is a recursive linear integration procedure. The total order of a one-sided problem is $G \times m!$, where G is the number of grid points for integration.

The two-sided probability

$$F_m(\mathbf{d}, \mathbf{c}) = \mathbb{P}\{d_i \leq X_i \leq c_i; 1 \leq i \leq m\}$$

can be calculated from 2^m m-dimensional one-sided probabilities which have the same mean and correlation matrix. The total order of this two-sided problem is $G \times m! \times 2^m$.

A new `algorithm` argument to `pmvnorm()` and `qmvnorm()` has been introduced in **mvtnorm** version 0.9-0 in order to switch between two algorithms: `GenzBretz()` is the default and triggers the use of the above mentioned quasi-randomized Monte-Carlo procedure by Genz and Bretz (1999). Alternatively, `algorithm = Miwa()` applies the procedure discussed here. Both functions can be used to specify hyper-parameters of the algorithm. For `Miwa()`, the argument `steps` defines the number of grid points G to be evaluated.

The following example shows how to calculate the probability

$$\begin{aligned} p &= F_m(\mathbf{d}, \mathbf{c}) \\ &= \mathbb{P}\{-1 < X_1 < 1, -4 < X_2 < 4, -2 < X_3 < 2\}. \end{aligned}$$

with mean $\mu = (0,0,0)^\top$ and correlation matrix

$$\mathbf{R} = \begin{pmatrix} 1 & 1/4 & 1/5 \\ 1/4 & 1 & 1/3 \\ 1/5 & 1/3 & 1 \end{pmatrix}$$

by using the following R code:

```
> library("mvtnorm")
> m <- 3
> S <- diag(m)
> S[2, 1] <- S[1, 2] <- 1 / 4
> S[3, 1] <- S[3, 1] <- 1 / 5
> S[3, 2] <- S[3, 2] <- 1 / 3
> pmvnorm(lower = -c(1,4,2),
+         upper = c(1,4,2),
+         mean=rep(0, m), sigma = S,
+         algorithm = Miwa())

[1] 0.6536804
attr(,"error")
[1] NA
attr(,"msg")
[1] "Normal Completion"
```

The upper limit and lower limit of the integral region are passed by the vectors `upper` and `lower`. The mean vector and correlation matrix are given by the vector `mean` and the matrix `sigma`. From the result we know that $p = 0.6536804$ with given correlation matrix $\mathbf{R}$.

Accuracy and time consumption

In this section we compare the accuracy and time consumption of the R implementation of the algo-

Algorithm	$m=5$		$m=10$	
	$\rho=\frac{1}{2}$	$\rho=-\frac{1}{2}$	$\rho=\frac{1}{2}$	$\rho=-\frac{1}{2}$
Genz & Bretz ($\varepsilon=10^{-4}$)	0.08468833	0.001385620	0.008863600	2.376316×10^{-8}
Genz & Bretz ($\varepsilon=10^{-5}$)	0.08472561	**0.001390769**	0.008863877	2.319286×10^{-8}
Genz & Bretz ($\varepsilon=10^{-6}$)	**0.08472682**	0.001388424	**0.008862195**	2.671923×10^{-8}
Miwa ($G=128$)	0.08472222	0.001388889	0.008863235	2.505205×10^{-8}
Exact.	0.08472222	0.001388889	0.008863236	2.505211×10^{-8}

Table 1: Value of probabilities with tri-diagonal correlation coefficients, $\rho_{i,i\pm1}=2^{-1}, 1\le i\le m$ and $\rho_{i,j}=0, \forall|i-j|>1$.

rithm of Miwa et al. (2003) with the default procedure for approximating multivariate normal probabilities in **mvtnorm** by Genz and Bretz (1999). The experiments were performed using an Intel® Pentium® 4 processor with 2.8 GHz.

Probabilities with tri-diagonal correlation matrix

The exact value of $P_m(\mu,\mathbf{R})$ is known if $\mathbf{R}$ has some special structure. E.g., when $\mathbf{R}$ is a m-dimensional tri-diagonal correlation matrix with correlation coefficients

$$\rho_{i,j}=\begin{cases} 2^{-1} & j=i\pm1 \\ 0 & |i-j|>1 \end{cases} \quad 1\le i\le m$$

the value of $P_m(\mathbf{0},\mathbf{R})$ is $((1+m)!)^{-1}$ (Miwa et al., 2003). The accuracy of Miwa' algorithm ($G=128$ grid points) and the Genz & Bretz algorithm (with absolute error tolerance $\varepsilon=10^{-4},10^{-5},10^{-6}$) for probabilities with tri-diagonal correlation matrix are compared in Table 1. In each calculation we have results with small variance. The values which do not hold the tolerance error are marked with bold characters in the tables. When the dimension is larger than five, using Genz & Bretz' algorithm, it is hard to achieve an error tolerance smaller than 10^{-5}.

Orthant probabilities

When $\mathbf{R}$ is the correlation matrix with $\rho_{i,j}=2^{-1}, i\neq j$, the value of $P_m(\mathbf{0},\mathbf{R})$ is known to be $(1+m)^{-1}$ (Miwa et al., 2003). Accuracy and time consumption of Miwa's algorithm and Genz & Bretz' algorithm for this situation are compared in Table 2.

Time consumption

Miwa's algorithm is a numerical method which has advantages in achieving higher accuracy with less time consumption compared to the stochastic method. However, Miwa's algorithm has some disadvantages. When the dimension m increases, the time consumption of Miwa's algorithm increases dramatically. Moreover, it can not be applied to singular problems which are common in multiple testing problems, for example.

Conclusion

We have implemented an R interface to the procedure of Miwa et al. (2003) in the R package **mvtnorm**. For small dimensions, it is an alternative to quasi-randomized Monte-Carlo procedures which are used by default. For larger dimensions and especially for singular problems, the method is not applicable.

Bibliography

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Algorithm	m=5		m=9	
	$\rho=\frac{1}{2}$	sec.	$\rho=\frac{1}{2}$	sec.
Genz & Bretz ($\varepsilon=10^{-4}$)	0.1666398	0.029	0.09998728	0.231
Genz & Bretz ($\varepsilon=10^{-5}$)	0.1666719	0.132	0.09998277	0.403
Genz & Bretz ($\varepsilon=10^{-6}$)	0.1666686	0.133	0.09999726	0.431
Miwa ($G=128$)	0.1666667	0.021	0.09999995	89.921
Exact.	0.1666667		0.10000000	

Table 2: Accuracy and time consumption of centered orthant probabilities with correlation coefficients, $\rho_{i,j}=2^{-1}, i\neq j$

Dimension	Miwa ($G = 128$)		Genz & Bretz ($\varepsilon = 10^{-4}$)	
	Single	Double	Single	Double
$m = 5$	0.021	0.441	0.029	0.085
$m = 6$	0.089	8.731	0.089	0.149
$m = 7$	0.599	156.01	0.083	0.255
$m = 8$	9.956	4hours	0.138	0.233
$m = 9$	89.921	-	0.231	0.392

Table 3: Time consumption of non-centered orthant probabilities (measured in seconds).

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Xuefei Mi
Institut für Biostatistik
Leibniz Universität Hannover, Germany
mi@biostat.uni-hannover.de

Tetsuhisa Miwa
National Institute for Agro-Environmental Sciences
Kannondai, Japan
miwa@niaes.affrc.go.jp

Torsten Hothorn
Institut für Statistik
Ludwig-Maximilians-Universität München, Germany
Torsten.Hothorn@R-project.org