Truncated Multivariate Gaussian Distribution on a Simplex

Nicolas Dobigeon and Jean-Yves Tourneret
E-mail : {Nicolas.Dobigeon, Jean-Yves.Tourneret}@enseeiht.fr

TECHNICAL REPORT – 2007, January

IRIT/ENSEEIHT/TéSA, 2 rue Camichel, BP 7122, 31071 Toulouse cedex 7, France

I. Problem statement

Let $\mathbb{S}$ denote the following simplex:

$$\mathbb{S} = \left\{ \boldsymbol{\alpha} \middle| \alpha_r \geq 0,\ \forall r = 1, \ldots, R-1,\ \sum_{r=1}^{R-1} \alpha_r \leq 1 \right\}, \tag{1}$$

Let $\mathcal{N}_{\mathbb{S}}(\boldsymbol{A}, \boldsymbol{B})$ denote the truncated multivariate normal distribution defined on the simplex $\mathbb{S}$ with mean vector $\boldsymbol{A}$ and covariance matrix $\boldsymbol{B}$. The probability density function (pdf) of this truncated multivariate normal distribution denoted as $\phi_{\mathbb{S}}\left(\cdot|\boldsymbol{A}, \boldsymbol{B}\right)$ satisfies the following relation:

$$\phi_{\mathbb{S}}\left(\boldsymbol{\alpha}|\boldsymbol{A}, \boldsymbol{B}\right) \propto \phi(\boldsymbol{\alpha}|\boldsymbol{A}, \boldsymbol{B}) \mathbf{1}_{\mathbb{S}}(\boldsymbol{\alpha}), \tag{2}$$

where

- $\phi\left(\cdot|\boldsymbol{A}, \boldsymbol{B}\right)$ is the standard Gaussian pdf with mean vector $\boldsymbol{A}$ and covariance matrix $\boldsymbol{\Sigma}$,
- $\mathbf{1}_{\mathbb{S}}(\cdot)$ is the indicator function defined on $\mathbb{S}$,
- $\propto$ stands for "proportional to".

This paper proposed to evaluate the normalization constant of the centered multivariate truncated normal distribution $\mathcal{N}_{\mathbb{S}}\left(\mathbf{0}_{R-1}, \sigma_0^2 \mathbf{I}_{R-1}\right)$, where $\mathbf{0}_{R-1}$ is the vector made of $R-1$ zeros and $\mathbf{I}_{R-1}$ is the $(R-1) \times (R-1)$ identity matrix. This normalization constant, denoted $K_{\mathbb{S}}\left(\sigma_0^2\right)$, can be derived directly from the definition of $\phi_{\mathbb{S}}\left(\boldsymbol{\alpha}|\boldsymbol{A}, \boldsymbol{B}\right)$:

$$\phi_{\mathbb{S}}\left(\boldsymbol{\alpha}|\boldsymbol{A}, \boldsymbol{B}\right) = \frac{1}{K_{\mathbb{S}}\left(\sigma_0^2\right)} \exp\left[-\frac{\|\boldsymbol{\alpha}\|^2}{2\sigma_0^2}\right]. \tag{3}$$

Consequently, it can be written:

$$K_{\mathbb{S}}\left(\sigma_0^2\right) = \int_{\mathbb{S}} f_{\sigma_0^2}\left(\boldsymbol{\alpha}\right) d\boldsymbol{\alpha}, \tag{4}$$

with

$$\begin{cases} \boldsymbol{\alpha} = [\alpha_1, \ldots, \alpha_{R-1}]^{\mathsf{T}}, \\ f_{\sigma_0^2}(\boldsymbol{\alpha}) = \exp\left[\frac{\sum_{r=1}^{R-1} \alpha_r^2}{2\sigma_0^2}\right]. \end{cases} \tag{5}$$

II. Case $R = 2$

For $R = 2$, the pdf of the Gaussian distribution truncated on the simplex $\mathbb{S} = \{\alpha_1 | 0 \leq \alpha_1 \leq 1\}$ reduces to the two-sided truncated normal distribution. As an example, the pdf of such distribution with $\sigma_0^2 = 0.2$ is depicted in Figure 1.

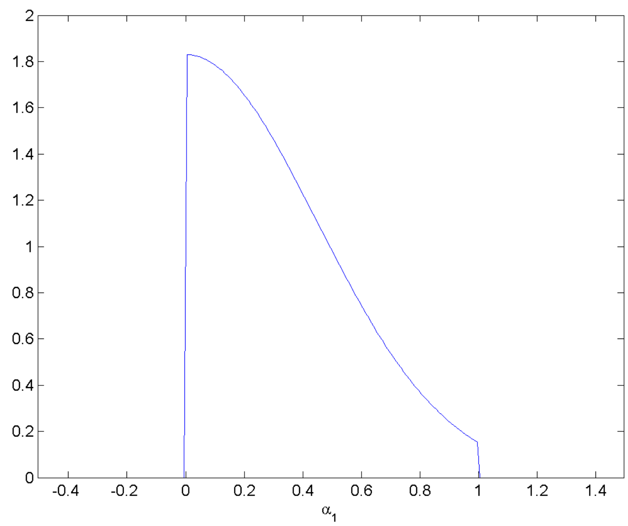

Fig. 1. Pdf of the normal distribution for $\sigma_0^2 = 0.2$ truncated on the simplex $\mathbb{S}$ ($R = 2$).

Consequently, the case $R = 2$ consists in computing the integral of the function $f_{\sigma_0^2}(\alpha_1) = \exp\left[-\frac{\alpha_1^2}{2\sigma_0^2}\right]$ on the set $\mathbb{S} = \{\alpha_1 | 0 \leq \alpha_1 \leq 1\}$:

$$K_{\mathbb{S}}\left(\sigma_0^2\right) = \int_0^1 \exp\left[-\frac{\alpha_1^2}{2\sigma_0^2}\right] d\alpha_1. \tag{6}$$

Let $t = \frac{\alpha_1}{\sqrt{2\sigma_0^2}}$,

$$K_{\mathbb{S}}\left(\sigma_0^2\right) = \sqrt{2\sigma_0^2} \int_0^{\frac{1}{\sqrt{2}\sigma_0}} \exp\left[-t^2\right] dt. \tag{7}$$

Finally,

$$\boxed{K_{\mathbb{S}}\left(\sigma_0^2\right) = \frac{\sqrt{2\pi\sigma_0^2}}{2} \operatorname{erf}\left(\frac{1}{\sqrt{2}\sigma_0}\right).} \tag{8}$$

III. CASE $R = 3$

For $R = 3$, the pdf of the multivariate Gaussian distribution with $\sigma_0^2 = 0.2$ truncated on the simplex $\mathbb{S}$ is depicted in Figure 2.

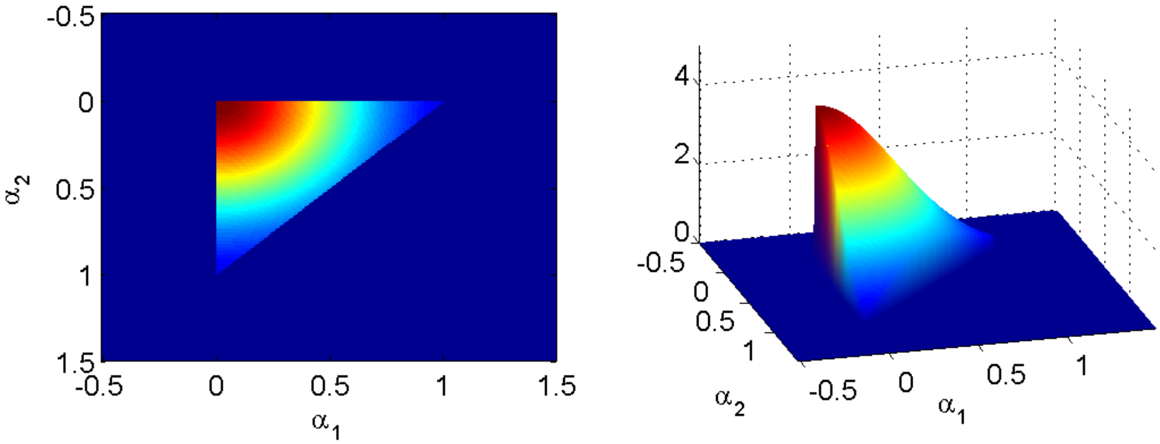

Fig. 2. Pdf of the multivariate Gaussian distribution for $\sigma_0^2 = 0.2$ truncated on the simplex $\mathbb{S}$ ($R = 3$).

Evaluating $K_{\mathbb{S}}\left(\sigma_0^2\right)$ consists in computing the integral of the function $f_{\sigma_0^2}\left(\boldsymbol{\alpha}\right) = \exp\left[-\frac{\alpha_1^2+\alpha_2^2}{2\sigma_0^2}\right]$ on the set represented in Figure 3 (left). As $f_{\sigma_0^2}\left(\boldsymbol{\alpha}\right)$ is even in α_1 and α_2, it can be written:

$$K_{\mathbb{S}}\left(\sigma_0^2\right) = \frac{1}{4}\int_{\mathbb{C}} \exp\left[-\frac{\alpha_1^2+\alpha_2^2}{2\sigma_0^2}\right] d\alpha_2 d\alpha_1. \tag{9}$$

where the set $\mathbb{C} = \left\{\boldsymbol{\alpha}\middle| |\alpha_1| + |\alpha_2| \leq 1\right\}$ is depicted in Figure 3 (right).

Moreover, the invariance by rotation of $f_{\sigma_0^2}\left(\boldsymbol{\alpha}\right)$ can be exploited. By denoting

$$\begin{bmatrix} u_1 \\ u_2 \end{bmatrix} = \begin{bmatrix} \cos(\theta) & \sin(\theta) \\ -\sin(\theta) & \cos(\theta) \end{bmatrix} \begin{bmatrix} \alpha_1 \\ \alpha_2 \end{bmatrix} \tag{10}$$

with $\theta = \frac{\pi}{4}$, it yields:

$$\begin{aligned} K_{\mathbb{S}}\left(\sigma_0^2\right) &= \frac{1}{4}\int_{-\frac{\sqrt{2}}{2}}^{\frac{\sqrt{2}}{2}}\int_{-\frac{\sqrt{2}}{2}}^{\frac{\sqrt{2}}{2}} \exp\left[-\frac{u_1^2+u_2^2}{2\sigma_0^2}\right] du_2 du_1 \\ &= \frac{1}{4}\left[\int_{-\frac{\sqrt{2}}{2}}^{\frac{\sqrt{2}}{2}} \exp\left[-\frac{u_1^2}{2\sigma_0^2}\right] du_1\right]^2 \\ &= \frac{1}{4}\left[2\int_{0}^{\frac{\sqrt{2}}{2}} \exp\left[-\frac{u_1^2}{2\sigma_0^2}\right] du_1\right]^2. \end{aligned} \tag{11}$$

Letting $t = \frac{u_1}{\sqrt{2\sigma_0^2}}$,

$$
\begin{aligned}
K_{\mathbb{S}}\left(\sigma_0^2\right) &= \frac{1}{4}\left[2\sqrt{2\sigma_0^2}\int_0^{\frac{1}{2\sigma_0}} \exp\left[-t^2\right] dt\right]^2 \\
&= 2\sigma_0^2 \left[\int_0^{\frac{1}{2\sigma_0}} \exp\left[-t^2\right] dt\right]^2 \\
&= 2\sigma_0^2 \left[\frac{\sqrt{\pi}}{2}\mathrm{erf}\left(\frac{1}{2\sigma_0}\right)\right]^2 .
\end{aligned}
\tag{12}
$$

Finally,

$$
\boxed{K_{\mathbb{S}}\left(\sigma_0^2\right) = \left[\frac{\sqrt{2\pi\sigma_0^2}}{2}\mathrm{erf}\left(\frac{1}{2\sigma_0}\right)\right]^2 .}
\tag{13}
$$

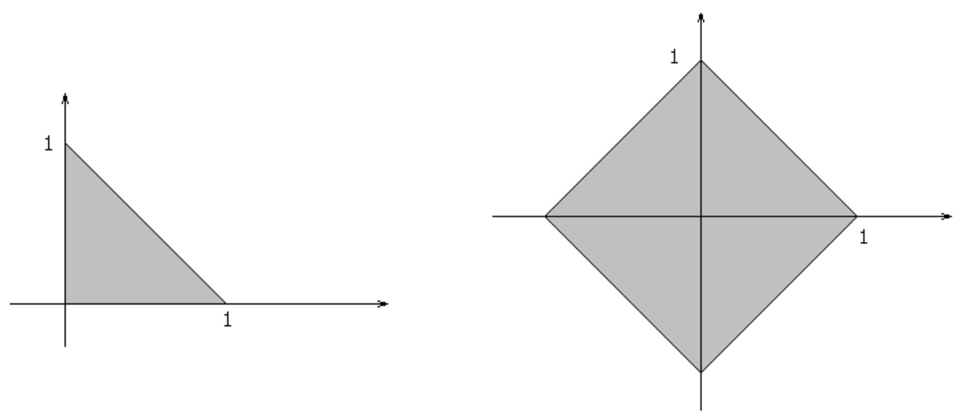

Fig. 3. The simplex $\mathbb{S}$ in $\mathbb{R}^2$ (left) and the set $\mathbb{C} = \left\{\boldsymbol{\alpha}\middle| |\alpha_1| + |\alpha_2| \leq 1\right\}$ (right).

IV. General case

The problem consists in computing the following quantity:

$$K_{\mathbb{S}}\left(\sigma_0^2\right) = \int_0^1 \int_0^{1-\alpha_1} \int_0^{1-\alpha_1-\alpha_2} \dots \int_0^{1-\sum_{r=1}^{R-2}\alpha_r} \exp\left[-\frac{\alpha_1^2 + \ldots + \alpha_{R-1}^2}{2\sigma_0^2}\right] d\alpha_{R-1} d\alpha_{R-2} \dots d\alpha_1, \tag{14}$$

that can be rewritten as:

$$\begin{aligned} K_{\mathbb{S}}\left(\sigma_0^2\right) = \int_0^1 \exp\left[-\frac{\alpha_1^2}{2\sigma_0^2}\right] \int_0^{1-\alpha_1} \exp\left[-\frac{\alpha_2^2}{2\sigma_0^2}\right] \int_0^{1-\alpha_1-\alpha_2} \dots \\ \dots \exp\left[-\frac{\alpha_{R-2}^2}{2\sigma_0^2}\right] \int_0^{1-\sum_{r=1}^{R-2}\alpha_r} \exp\left[-\frac{\alpha_{R-1}^2}{2\sigma_0^2}\right] d\alpha_{R-1} d\alpha_{R-2} \dots d\alpha_1. \end{aligned} \tag{15}$$

As in [1], we introduce:

$$\begin{aligned} g_{R-1}\left(y\right) &= \int_0^y \exp\left[-\frac{t^2}{2\sigma_0^2}\right] dt \\ &= \frac{\sqrt{2\pi\sigma_0^2}}{2} \operatorname{erf}\left(\frac{y}{\sqrt{2\sigma_0^2}}\right). \end{aligned} \tag{16}$$

Then outer integrals can be recursively defined by the following sequence of functions:

$$g_r\left(y\right) = \int_0^y \exp\left[-\frac{t^2}{2\sigma_0^2}\right] g_{r+1}\left(y-t\right) dt, \tag{17}$$

ending with

$$\boxed{K_{\mathbb{S}}\left(\sigma_0^2\right) = g_1(1)}. \tag{18}$$

V. Asymptotic behavior

When $\sigma_0 \to \infty$, i.e. $x = \frac{1}{\sqrt{2\sigma_0^2}} \to 0$, the normal distribution reduces to the uniform distribution on $\mathbb{S}$. As an example, the pdf of the multivariate Gaussian distribution for $\sigma_0^2 = 50$ truncated on the simplex defined in Eq. (1) is depicted in Figure 4 for $R = 3$.

For $R = 2$ or $R = 3$, approximations of the erf function leads to $K_{\mathbb{S}}\left(\sigma_0^2\right) = \frac{1}{(R-1)!}$ [2, p. 297]. This result can be easily generalized for $R > 3$. By using the first order approximation $\exp(x) = 1 + \mathrm{o}\left(\frac{1}{x^2}\right)$, Eq. (14) reduces to:

$$K_{\mathbb{S}}\left(\sigma_0^2\right) = \int_{\mathbb{S}} d\boldsymbol{\alpha} = \mathrm{vol}\left(\mathbb{S}\right), \tag{19}$$

where $\mathrm{vol}\left(\cdot\right)$ stands for the volume. In the case of the simplex defined in Eq. (1), $\mathrm{vol}\left(\mathbb{S}\right) = \frac{1}{(R-1)!}$.

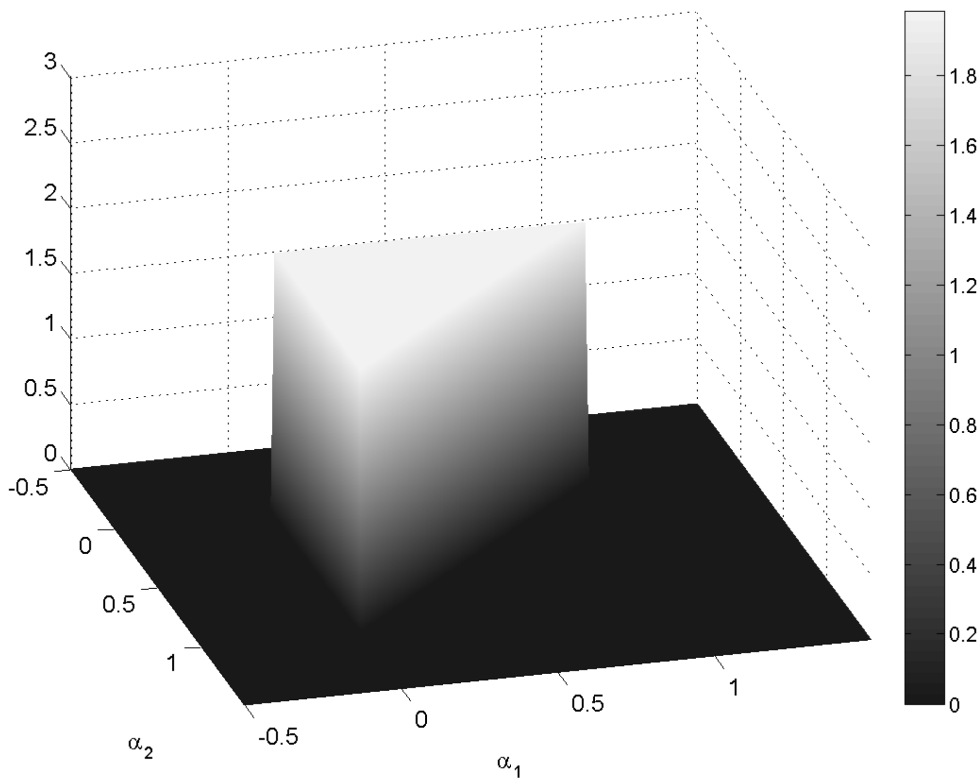

Fig. 4. Pdf of the multivariate Gaussian distribution for $\sigma_0^2 = 50$ truncated on the simplex $\mathbb{S}$ ($R = 3$).

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[1] A. Genz and P. Joyce, "Computation of the normalization constant for exponentially weighted dirichlet distribution integrals," *Computing Science and Statistics*, vol. 35, pp. 557–563, 2003.

[2] M. Abramowitz and I. A. Stegun, *Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables*, ninth Dover printing, tenth GPO printing ed. New York: Dover, 1964.