MATHEMATICAL COMMUNICATIONS
Math. Commun. **18**(2013), 349–358

Integration of positive linear functionals on a sphere in $\mathbb{R}^{2n}$ with respect to Gaussian surface measures

Ivica Nakić[1,*]

[1] *Department of Mathematics, University of Zagreb, Bijenička 30, HR-10 000 Zagreb, Croatia*

Received September 12, 2012; accepted May 4, 2013

Abstract. In this paper we present a formula for the calculation of the integrals of the form $\int_S u^* X u \, \nu(\mathrm{d}u)$, where S is the unit sphere in $\mathbb{R}^N$, X is a positive semi-definite symmetric matrix, and ν is a surface measure generated by a Gaussian measure μ. The solution has the form trace(XZ), with the explicit procedure for the calculation of the matrix Z which does not depend on X.

AMS subject classifications: 28A25, 58D20

Key words: integration on a sphere, surface measure

1. Introduction

Our aim in this paper is to give an explicit procedure for the calculation of the integrals of the form

$$\int_S u^* X u \, \nu(\mathrm{d}u), \tag{1}$$

where S is the unit sphere in $\mathbb{R}^N$, X is a positive semi-definite symmetric matrix, and ν is a surface measure generated by a Gaussian measure μ. Here u^* denotes the transpose of u. More precisely, for the measure ν we take the measure induced by the Gaussian measure μ via Minkowski formula (see [1]):

$$\int_S f \mathrm{d}\nu = \lim_{\varepsilon \to 0} \frac{1}{2\varepsilon} \int_{d(x,S) \leq \varepsilon} f(x) \mu(\mathrm{d}x). \tag{2}$$

We assume that the measure μ has zero mean and covariance matrix K with all non-zero eigenvalues having even multiplicities. This is satisfied if, for example, the covariance matrix has the form $K = \mathrm{diag}(\tilde{K}, \tilde{K})$. Our assumption on K is natural in cases of systems which are linearizations of second order systems.

Our main motivation for the calculation of these types of integrals comes from the optimal control. Let us assume that we wish to minimize some quantity of a dynamical system which depends on the initial state. To make this procedure independent of the initial conditions, we can try to minimize the average of our quantity over all initial states of the unit norm. If our quantity can be expressed in the form $u^* X u$, for some positive semi-definite symmetric matrix (for example,

*Corresponding author. *Email address:* `nakic@math.hr` (I. Nakić)

the total energy), then we end up with (1). Since (1) defines a linear functional on the space of symmetric matrices, Riesz representation theorem (see, for example [4]) implies the existence of the positive semi-definite symmetric matrix Z such that

$$\int_S u^* X u \, \nu(\mathrm{d}u) = \mathrm{tr}(XZ), \tag{3}$$

where Z depends only on the choice of the measure μ. Hence, if we find the formula for the matrix Z, we can calculate (1).

2. Main result

We decompose $\mathbb{R}^N$ into $\mathbb{R}^N = Y_1 \oplus Y_2$, where Y_2 is the null-space of the operator K, and Y_1 is the orthogonal complement of Y_2. Then $\mu_Y = \mu_{Y_1} \times \mu_{Y_2}$, where μ_{Y_1} is a Gaussian measure with zero mean and covariance operator $P_{Y_1} K P_{Y_1}$, P_{Y_1} being the orthogonal projector in Y_1, and μ_{Y_2} is a Dirac measure in Y_2 concentrated at zero (in other words, a Gaussian measure with zero mean and zero covariance).

Let us fix a basis in $\mathbb{R}^N$ such that K has a matrix representation of the form

$$K = \begin{bmatrix} K_1 & 0 \\ 0 & 0 \end{bmatrix},$$

$K_1 \in \mathbb{R}^{2t \times 2t}$ being positive definite. Then it follows that Z has the matrix representation

$$Z = \begin{bmatrix} Z_1 & 0 \\ 0 & 0 \end{bmatrix}. \tag{4}$$

Indeed, let E_{ij} denote the matrix which has all entries zero except for the entry (i, j) which has value 1. Let $X = (X_{ij})$ be an arbitrary symmetric matrix in $\mathbb{R}^N$. We have

$$\begin{aligned} \mathrm{tr}(XZ) &= \sum_{i,j} X_{ij} \, \mathrm{tr}(Z E_{ij}) = \sum_{i,j} X_{ij} \int_S x^* E_{ij} x \, \nu(\mathrm{d}x) \\ &= \sum_{i,j} X_{ij} \int_S x_i x_j \, \nu(\mathrm{d}x), \end{aligned}$$

hence

$$Z_{ij} = \int_S x_i x_j \, \nu(\mathrm{d}x). \tag{5}$$

To obtain (4) we just have to take into account the structure of the covariance matrix K and Minkowski formula (2).

Therefore, our aim is to compute the matrix Z_1, where Z_1 is such that (3) holds for the measure ν_{Y_1} in Y_1, since ν_{Y_2} is everywhere zero.

Lemma 1. *The following formula holds*

$$\int_{S_{Y_1}} \mathrm{d}\nu_{Y_1} = \frac{\mathrm{d}}{\mathrm{d}r}\bigg|_{r=1} \left(\int_{x^* x \le r^2} \mu_{Y_1}(\mathrm{d}x) \right). \tag{6}$$

Proof. Let us define the function

$$g(r) = \int_{x^*x \le r^2} \mu_{Y_1}(\mathrm{d}x).$$

The function g is an analytic function [3, Corollary 3.4] (we will later explicitly calculate the function g), and the left-hand side in (6) can be written as

$$\int_{S_{Y_1}} \mathrm{d}\nu_{Y_1} = \lim_{\varepsilon\to 0}\frac{1}{2\varepsilon}\int_{d(x,S)\le\varepsilon}\mu_{Y_1}(\mathrm{d}x) = \lim_{\varepsilon\to 0}\frac{g(1+\varepsilon)-g(1-\varepsilon)}{2\varepsilon}$$
$$= \lim_{\varepsilon\to 0}\frac{1}{2}\left(\frac{g(1+\varepsilon)-g(1)}{\varepsilon}+\frac{g(1)-g(1-\varepsilon)}{\varepsilon}\right) = g'(1).$$

□

The density function of μ_{Y_1} with respect to the Lebesgue measure is

$$p(x) = \frac{1}{(2\pi)^t\sqrt{\det K_1}}e^{-1/2x^*K_1{}^{-1}x},$$

hence

$$\int_{x^*x\le r^2}\mu_{Y_1}(\mathrm{d}x) = \frac{1}{(2\pi)^t\sqrt{\det K_1}}\int_{x^*x\le r^2}e^{-1/2x^*K_1{}^{-1}x}\mathrm{d}x. \tag{7}$$

Let $K_1 = LL^*$ be a Cholesky factorization of K_1, and let $L^*L = U^*\Lambda U$ be a spectral decomposition of L^*L, where $\Lambda = \mathrm{diag}(\mu_1,\dots,\mu_{2t})$. Note that $\mu_1,\dots,\mu_{2t}$ are eigenvalues of K_1. By means of the substitution $x = LU^*y$, from (7) we obtain

$$\int_{x^*x\le r^2}\mu_{Y_1}(\mathrm{d}x) = \frac{1}{(2\pi)^t}\int_{y^*\Lambda y\le r^2}e^{-1/2y^*y}\mathrm{d}y = \mathbb{P}\{\sum_{j=1}^{2t}\mu_j\mathbb{X}_j^2 \le r^2\}, \tag{8}$$

where $\mathbb{X}_i \sim N(0,1)$ are Gaussian random vectors with zero mean and the unit covariance matrix, and $\mathbb{P}$ denotes the probability. Hence (see, for example [2, p. 48]), follows

$$\mathbb{P}\{\sum_{j=1}^{2t}\mu_jX_j^2\le r^2\} = \mathbb{P}\{\sum_{j=1}^{2t}\mu_j\chi_j(1)\le r^2\} = \mathbb{P}\{\sum_{j=1}^{m}\lambda_j\chi_j(k_j)\le r^2\}, \tag{9}$$

where $\chi(k)$ denotes the chi-squared distribution with k degrees of freedom, m is the number of eigenvalues not taking into account multiplicities, and by $\lambda_1,\dots,\lambda_m$ we denoted mutually different eigenvalues of K_1, with their multiplicities k_j. Here we can assume that $\chi_j(k_j)$ are independent random variables.

From our assumption on the covariance matrix K we know that k_j are always even, which we will need to obtain (12).

Let us denote by f and φ the probability density function and the characteristic function of $\sum_{j=1}^m\lambda_j\chi_j(k_j)$, respectively. Then [2, Chapter 15.]

$$\mathbb{P}\{\sum_{j=1}^{m}\lambda_j\chi_j(k_j)\le r^2\} = \int_0^{r^2}f(x)\mathrm{d}x, \tag{10}$$

hence (6), (8), (9) and (10) imply

$$\int_{S_{Y_1}} \mathrm{d}\nu_{Y_1} = 2f(1). \tag{11}$$

From [2, Chapter 15] also follows

$$\varphi(t) = \prod_{j=1}^{m} \varphi_{\chi_j(k_j)}(\lambda_j t) = \prod_{j=1}^{m} (1-2it\lambda_j)^{-k_j/2}.$$

Set $g_j = \frac{k_j}{2}$. We want to expand $\varphi(t)$ in partial fractions, i.e. to obtain

$$\prod_{j=1}^{m} (1-2it\lambda_j)^{-g_j} = \sum_{j=1}^{m}\sum_{s=1}^{g_j} \alpha_{js}(1-2it\lambda_j)^{-s}. \tag{12}$$

To calculate the coefficients α_{js} we proceed as follows. Fix $k \in \{1,\dots,m\}$. We can rewrite (12) as

$$(1-2it\lambda_k)^{-g_k}\prod_{j\neq k}(1-2it\lambda_j)^{-g_j} = \sum_{s=1}^{g_k}\alpha_{ks}(1-2it\lambda_k)^{-s} + \sum_{j\neq k}^{m}\sum_{w=1}^{g_j}\alpha_{jw}(1-2it\lambda_j)^{-w}.$$

Multiplying the previous relation by $(1-2it\lambda_k)^{g_k}$, and substituting $y = 1-2it\lambda_k$ we get

$$\prod_{j\neq k}\left(\frac{\lambda_k-\lambda_j}{\lambda_k} + y\frac{\lambda_j}{\lambda_k}\right)^{-g_j} = \sum_{s=1}^{g_k}\alpha_{ks}y^{g_k-s} + y^{g_k}\sum_{j\neq k}^{m}\sum_{w=1}^{g_j}\alpha_{jw}\left(\frac{\lambda_k-\lambda_j}{\lambda_k} + y\frac{\lambda_j}{\lambda_k}\right)^{-w}. \tag{13}$$

We can look at (13) as an equality of two rational functions on the line $1+i\mathbb{R}$. But this equality can be extended to all complex numbers for which (13) makes sense. Indeed, (13) can be written as

$$\frac{p_1(y)}{q_1(y)} = \frac{p_2(y)}{q_2(y)},$$

where p_1, p_2, q_1 and q_2 are polynomials, hence holomorphic functions on $\mathbb{C}$. But this implies $p_1q_2 = p_2q_1$, which is an equality of two holomorphic functions on the line. This implies that (13) holds everywhere except at the zeros of q_1 and q_2.

So we can take $y = 0$ in (13) and obtain

$$\alpha_{ig_i} = \prod_{j\neq i}\left(\frac{\lambda_i-\lambda_j}{\lambda_i}\right)^{-g_j}.$$

Our next step is to calculate the rest of the coefficients α_{ij}. When we differentiate both sides of (13) k times ($k = 1,\dots,g_i-1$) and take $y = 0$, we obtain

$$\alpha_{i,g_i-k} = \frac{f_i^{(k)}(0)}{k!}, \text{ where } f_i(y) = \prod_{j\neq i}\left(\frac{\lambda_i-\lambda_j}{\lambda_i} + y\frac{\lambda_j}{\lambda_i}\right)^{-g_j}.$$

Set

$$\psi_i(y) = \ln f_i(y) = -\sum_{j\neq i} g_j \ln \left| \frac{\lambda_i - \lambda_j}{\lambda_i} + y\frac{\lambda_j}{\lambda_i} \right|.$$

We calculate the derivatives in zero of the functions ψ_i and obtain

$$\psi_i^{(k)}(0) = (-1)^k (k-1)! \sum_{j\neq i} \frac{g_j}{\left|\frac{\lambda_i}{\lambda_j} - 1\right|^k} \quad \text{for } k \geq 1.$$

Now we can calculate derivatives in zero of the functions f_i by using the following recursive procedure:

$$\begin{aligned} f_i^{(1)}(0) &= f_i(0)\psi_i^{(1)}(0), \\ f_i^{(k+1)}(0) &= \sum_{l=0}^{k} \binom{k}{l} f_i^{(k-l)}(0)\psi_i^{(l+1)}(0),\ k = 2, \ldots, g_i - 1. \end{aligned}$$

After a straightforward calculation we get the following recursive formula for the coefficients α_{ij}, $i = 1, \ldots, m$:

$$\begin{aligned} \alpha_{ig_i} &= \prod_{j\neq i} \left(1 - \frac{\lambda_j}{\lambda_i}\right)^{-g_j}, \\ \alpha_{i,g_i-1} &= -\alpha_{ig_i} \sum_{j\neq i} \frac{g_j}{\left|\frac{\lambda_i}{\lambda_j} - 1\right|}, \\ \alpha_{i,g_i-k-1} &= \frac{1}{k+1} \sum_{l=0}^{k} (-1)^{l+1} \alpha_{i,g_i-k+l} \sum_{j\neq i} \frac{g_j}{\left|\frac{\lambda_i}{\lambda_j} - 1\right|^{l+1}},\ k = 1, 2, \ldots, g_i - 2. \end{aligned} \tag{14}$$

Since $f(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{-itx}\varphi(t)\mathrm{d}t$, we have

$$f(x) = \sum_{j=1}^{m} \sum_{l=1}^{g_j} \alpha_{jl} f_{\lambda_j \chi(2l)}(x).$$

Now the last equation, together with (11), implies

$$\begin{aligned} \int_{S_Y} \mathrm{d}\nu_Y &= 2\sum_{j=1}^{m}\sum_{l=1}^{g_j} \alpha_{jl} f_{\lambda_j\chi(2l)}(1) = 2\sum_{j=1}^{m}\sum_{l=1}^{g_j} \alpha_{jl} \frac{1}{\lambda_j} f_{\chi(2l)}\left(\frac{1}{\lambda_j}\right) \\ &= 2\sum_{j=1}^{m}\sum_{l=1}^{g_j} \alpha_{jl} \frac{1}{\lambda_j^l} \frac{1}{2^l (l-1)!} e^{-\frac{1}{2\lambda_j}} = 2\sum_{j=1}^{m} e^{-\frac{1}{2\lambda_j}} \sum_{l=1}^{g_j} \alpha_{jl} \frac{1}{\lambda_j^l} \frac{1}{2^l (l-1)!}, \end{aligned} \tag{15}$$

since the probability density function of the chi-squared distribution with k degrees of freedom is given by

$$f_{\chi(k)}(x) = \frac{1}{2^{k/2}\Gamma(k/2)} e^{-\frac{x}{2}} x^{k/2-1}.$$

Hence we have found a recursive formula for the calculation of the surface measure of the sphere. It turns out that we can also calculate the entries of the matrix Z_1 by using the coefficients α_{ij}.

From (5) it follows

$$(Z_1)_{ij} = \int_{S_{Y_1}} x_i x_j \, \nu_{Y_1}(\mathrm{d}x). \tag{16}$$

Let ${K_1}^{-1} = V\Lambda V^*$ be a spectral decomposition of the operator ${K_1}^{-1}$, with V orthogonal matrix. By using (2) and substituting $x = Vy$, we obtain

$$\begin{aligned}\int_{S_{Y_1}} x_i x_j \, \nu_{Y_1}(\mathrm{d}x) &= \frac{1}{(2\pi)^t \sqrt{\det K_1}} \lim_{\varepsilon\to 0} \frac{1}{2\varepsilon} \int_{d(x,S_{Y_1})\le\varepsilon} x_i x_j e^{-1/2x^* {K_1}^{-1} x} \mathrm{d}x \\ &= \frac{1}{(2\pi)^t \sqrt{\det K_1}} \lim_{\varepsilon\to 0} \frac{1}{2\varepsilon} \int_{d(x,S_{Y_1})\le\varepsilon} (Vy)_i (Vy)_j e^{-1/2y^*\Lambda y} \mathrm{d}y.\end{aligned} \tag{17}$$

Since $(Vy)_i(Vy)_j = y^* \widetilde{E}_{ij} y$, where

$$\widetilde{E}_{ij} = V^* E_{ij} V, \tag{18}$$

to compute $(Z_1)_{ij}$ it is enough to calculate

$$\lim_{\varepsilon\to 0} \frac{1}{2\varepsilon} \int_{d(x,S_{Y_1})\le\varepsilon} y_i y_j e^{-1/2y^*\Lambda y} \mathrm{d}y. \tag{19}$$

To calculate (19) we use the (generalized) spherical coordinates:

$$\begin{aligned}\int_{d(x,S_{Y_1})\le\varepsilon} y_i y_j e^{-1/2y^*\Lambda y} \mathrm{d}y = &\int_{1-\varepsilon}^{1+\varepsilon} \mathrm{d}\rho \int_0^\pi \mathrm{d}\phi_1 \cdots \int_0^\pi \mathrm{d}\phi_{2t-2} \\ &\times \int_0^{2\pi} \mathrm{d}\phi_{2t-1} y_i y_j e^{-1/2y^*\Lambda y} \rho^{2t-1} \sin^{2t-2}\phi_1 \cdots \sin\phi_{2t-2},\end{aligned}$$

where $y_i = \rho \sin\phi_1 \cdots \sin\phi_{i-1} \cos\phi_i$, $i = 1, \ldots, 2t-1$ and $y_{2t} = \rho \sin\phi_1 \cdots \sin\phi_{2t-1}$. If we denote the last $2t-1$ integrals in the previous relation by $g(\rho)$, then

$$\lim_{\varepsilon\to 0} \frac{1}{2\varepsilon} \int_{d(x,S_{Y_1})\le\varepsilon} y_i y_j e^{-1/2y^*\Lambda y} \mathrm{d}y = \lim_{\varepsilon\to 0} \frac{1}{2\varepsilon} \int_{1-\varepsilon}^{1+\varepsilon} g(\rho) \mathrm{d}\rho = g(1),$$

where we used the same procedure as in Lemma 1. Hence (19) is equal to

$$\int_{S_{Y_1}} y_i y_j e^{-1/2y^*\Lambda y} \mathrm{d}y.$$

Note that this integral equals zero in the case $i \ne j$.

Analogously we obtain

$$\int_{S_{Y_1}} \mathrm{d}\nu_{Y_1} = \frac{1}{(2\pi)^t \sqrt{\det K_1}} \int_{S_{Y_1}} e^{-1/2y^*\Lambda y} \mathrm{d}y. \tag{20}$$

Let $\xi : \{1,\dots,2t\} \to \{1,\dots,m\}$ be the function such that $\xi(i) = j$ implies $\mu_i = \lambda_j$. Let us fix $i \in \{1,\dots,2t\}$. Due to the symmetry of the measure ν_{Y_1}, we have

$$\int_{S_{Y_1}} x_i^2 \nu_{Y_1}(\mathrm{d}x) = \int_{S_{Y_1}} x_j^2 \nu_{Y_1}(\mathrm{d}x) \tag{21}$$

for all $j \in \xi^{-1}(\xi(i))$.

Because of (20) we can interpret $\int_{S_{Y_1}} \mathrm{d}\nu_{Y_1}$ as a function in the variables $\lambda_1,\dots,\lambda_m$, i.e. we denote

$$F(\lambda_1,\dots,\lambda_m) = \frac{1}{(2\pi)^t\sqrt{\det K_1}} \int_{S_{Y_1}} e^{-1/2\sum_{i=1}^m \lambda_i \sum_{j\in\xi^{-1}(\xi(i))} y_j^2} \mathrm{d}y.$$

All partial derivatives of this function exist and

$$\frac{\partial}{\partial\lambda_i} F(\lambda_1,\dots,\lambda_m) = -\frac{1}{2}\frac{1}{(2\pi)^t\sqrt{\det K_1}} \int_{S_{Y_1}} \sum_{j\in\xi^{-1}(\xi(i))} y_j^2 e^{-1/2y^*\Lambda y}\mathrm{d}y.$$

The last relation, together with (21), implies

$$\int_{S_{Y_1}} y_i^2 e^{-1/2y^*\Lambda y}\mathrm{d}y = -2\frac{(2\pi)^t\sqrt{\det K_1}}{k_{\xi(i)}} \frac{\partial}{\partial\lambda_{\xi(i)}} F(\lambda_1,\dots,\lambda_m). \tag{22}$$

Hence, the relations (16), (17), (20), (21), and (22) imply

$$(Z_1)_{ij} = -2\sum_l \frac{(\widetilde{E}_{ij})_{ll}}{k_{\xi(l)}} \frac{\partial}{\partial\lambda_{\xi(l)}} F(\lambda_1,\dots,\lambda_m), \tag{23}$$

where $\widetilde{E}_{ij}$ is given by (18).

From (15) it follows

$$F(\lambda_1,\dots,\lambda_m) = 2\sum_{j=1}^m e^{-\frac{1}{2\lambda_j}} \sum_{l=1}^{g_j} \alpha_{jl}\frac{1}{\lambda_j^l 2^l(l-1)!},$$

where α_{jl} is interpreted as a function in variables $\lambda_1,\dots,\lambda_m$. We calculate

$$\begin{aligned}\frac{\partial}{\partial\lambda_i} F(\lambda_1,\dots,\lambda_m) = 2\sum_{j=1}^m e^{-\frac{1}{2\lambda_j}} \sum_{l=1}^{g_j} \frac{\frac{\partial}{\partial\lambda_i}\alpha_{jl}}{\lambda_j^l}\frac{1}{2^l(l-1)!} + \frac{1}{\lambda_i^2} e^{-\frac{1}{2\lambda_i}} \sum_{l=1}^{g_i} \frac{\alpha_{il}}{\lambda_i^l}\frac{1}{2^l(l-1)!} \\ - 2e^{-\frac{1}{2\lambda_i}} \sum_{l=1}^{g_i} \frac{l\alpha_{il}}{\lambda_i^{l+1}}\frac{1}{2^l(l-1)!}.\end{aligned} \tag{24}$$

Since $\alpha_{jl} = \frac{f_j^{(g_j-l)}(0)}{(g_j-l)!}$, we have

$$\frac{\partial}{\partial\lambda_i}\alpha_{jl} = \frac{1}{(g_j-l)!}\frac{\partial}{\partial y^{g_j-l}}\frac{\partial}{\partial\lambda_i} f_j(y,\lambda_1,\dots,\lambda_m)\bigg|_{y=0},$$

where f_j is taken as a function in variables $y, \lambda_1, \dots, \lambda_m$. Now

$$\begin{aligned}\frac{\partial}{\partial \lambda_i} f_j(y, \lambda_1, \dots, \lambda_m) &= f_j(y, \lambda_1, \dots, \lambda_m) \frac{\partial}{\partial \lambda_i} \ln f_j(y, \lambda_1, \dots, \lambda_m) \\ &= -f_j(y, \lambda_1, \dots, \lambda_m) \sum_{l \neq j} g_l \frac{\partial}{\partial \lambda_i} \ln \left| \frac{\lambda_j - \lambda_l}{\lambda_j} + y \frac{\lambda_l}{\lambda_j} \right|.\end{aligned}$$

In the case $i \neq j$ we obtain

$$\frac{\partial}{\partial \lambda_i} f_j(y, \lambda_1, \dots, \lambda_m) = -f_j(y, \lambda_1, \dots, \lambda_m) \frac{g_i(y-1)}{\lambda_j - \lambda_i + y\lambda_i},$$

and in the case $i = j$ we obtain

$$\frac{\partial}{\partial \lambda_i} f_i(y, \lambda_1, \dots, \lambda_m) = f_i(y, \lambda_1, \dots, \lambda_m) \frac{y-1}{\lambda_i} \sum_{l \neq i} \frac{g_l \lambda_l}{\lambda_i - \lambda_l + y\lambda_l}.$$

Let us define functions $\phi_{ji}(y) = \frac{g_i(y-1)}{\lambda_j - \lambda_i + y\lambda_i}$. From the straightforward calculation we obtain:

$$\phi_{ji}^{(k)}(0) = \frac{(-1)^{k-1} k! g_i \lambda_j \lambda_i^{k-1}}{(\lambda_j - \lambda_i)^{k+1}}, \text{ for } k > 0 \text{ and } \phi_{ji}(0) = -\frac{g_i}{\lambda_j - \lambda_i}.$$

Hence in the case $i \neq j$ we have

$$\begin{aligned}\frac{\partial}{\partial \lambda_i} \alpha_{jl} &= -\frac{1}{(g_j - l)!} \sum_{k=0}^{g_j - l} \binom{g_j - l}{k} f_j^{(g_j - l - k)}(0) \phi_{ji}^{(k)}(0) \\ &= g_i \left(\frac{\alpha_{jl}}{\lambda_j - \lambda_i} + \lambda_j \sum_{k=1}^{g_j - l} (-1)^k \frac{\lambda_i^{k-1} \alpha_{j,l+k}}{(\lambda_j - \lambda_i)^{k+1}} \right) \\ &= g_i \left(\frac{\alpha_{jl}}{\lambda_j - \lambda_i} + \frac{\lambda_j}{\lambda_i(\lambda_j - \lambda_i)} \sum_{k=1}^{g_j - l} (-1)^k \left(\frac{\lambda_i}{\lambda_j - \lambda_i} \right)^k \alpha_{j,l+k} \right).\end{aligned} \tag{25}$$

For the case $i = j$, let us define $\phi_i(y) = \frac{y-1}{\lambda_i} \sum_{p \neq i} \frac{g_p \lambda_p}{\lambda_i - \lambda_p + y\lambda_p}$. Then

$$\phi_i^{(k)}(0) = (-1)^{k-1} k! \sum_{p \neq i} \frac{g_p \lambda_p^k}{(\lambda_i - \lambda_p)^{k+1}}, \text{ for } k > 0 \text{ and } \phi_i(0) = -\frac{1}{\lambda_i} \sum_{p \neq i} \frac{g_p \lambda_p}{\lambda_i - \lambda_p}.$$

Hence

$$\begin{aligned}\frac{\partial}{\partial \lambda_i} \alpha_{il} &= \frac{1}{(g_i - l)!} \sum_{k=0}^{g_i - l} \binom{g_i - l}{k} f_i^{(g_i - l - k)}(0) \phi_i^{(k)}(0) \\ &= -\frac{\alpha_{il}}{\lambda_i} \sum_{p \neq i} \frac{g_p \lambda_p}{\lambda_i - \lambda_p} - \sum_{k=1}^{g_i - l} (-1)^k \alpha_{i,l+k} \sum_{p \neq i} \frac{g_p \lambda_p^k}{(\lambda_i - \lambda_p)^{k+1}}.\end{aligned} \tag{26}$$

If we insert (25) and (26) into (24), we obtain

$$\frac{\partial}{\partial\lambda_i}F(\lambda_1,\ldots,\lambda_m)=\sum_{j=1}^{m}\sum_{l=1}^{g_j}\beta_{ijl}\alpha_{jl}, \tag{27}$$

where in the case $i\neq j$, $l=1$ we have

$$\beta_{ij1}=e^{-\frac{1}{2\lambda_j}}\frac{g_i}{\lambda_j(\lambda_j-\lambda_i)}, \tag{28}$$

and in the case $i\neq j$, $l\neq 1$

$$\beta_{ijl}=2g_i\frac{e^{-\frac{1}{2\lambda_j}}}{\lambda_j-\lambda_i}\left(\frac{1}{2^l(l-1)!}\frac{1}{\lambda_j^l}+\frac{\lambda_j}{\lambda_i}\sum_{k=1}^{l-1}(-1)^{l-k}\left(\frac{\lambda_i}{\lambda_j-\lambda_i}\right)^{l-k}\frac{1}{\lambda_j^k}\frac{1}{2^k(k-1)!}\right). \tag{29}$$

In the case $i=j$ we have

$$\beta_{ii1}=\frac{e^{-\frac{1}{2\lambda_i}}}{\lambda_i^2}\left(\frac{1}{2\lambda_i}-1-\sum_{p\neq i}\frac{g_p\lambda_p}{\lambda_i-\lambda_p}\right), \tag{30}$$

and for $l\neq 1$ we have

$$\begin{aligned}\beta_{iil}=e^{-\frac{1}{2\lambda_i}}&\frac{1}{\lambda_i^{l+1}}\frac{1}{2^l(l-1)!}\left(\frac{1}{\lambda_i}-2l-2\sum_{p\neq i}\frac{g_p\lambda_p}{\lambda_i-\lambda_p}\right)\\&-2e^{-\frac{1}{2\lambda_i}}\sum_{k=1}^{l-1}\frac{1}{\lambda_i^k}\frac{1}{2^k(k-1)!}(-1)^{l-k}\sum_{p\neq i}\frac{g_p\lambda_p^{l-k}}{(\lambda_i-\lambda_p)^{l-k+1}}.\end{aligned} \tag{31}$$

For example, to obtain (28), we have to find the coefficient of α_{ji} in (24), which is

$$2e^{-\frac{1}{2\lambda_j}}\frac{1}{\lambda_j}\frac{1}{2}g_i\frac{\alpha_{j1}}{\lambda_j-\lambda_i},$$

which gives (28).

Hence the procedure of the computation of the entries of the matrix Z_1 consists of four steps:

(i) compute the coefficients α_{ij} using formulae (14);

(ii) compute the coefficients β_{ijl} using (28), (29), (30) and (31);

(iii) compute $\frac{\partial}{\partial\lambda_i}F(\lambda_1,\ldots,\lambda_m)$ using (27);

(iv) compute $(Z_1)_{ij}$ using (23).

This algorithm is numerically unstable in the case in which g_i's are large because the expression for α_{ig_i} contains the potential $-g_i$. Since the expression $\lambda_i-\lambda_j$ appears in the denominator of the expressions for α_{ij}'s and β_{ijl}'s, if λ_i is close to λ_j for some $i \neq j$, the algorithm will also be numerically unstable.

In such cases one can use a Monte Carlo method of numerical integration to compute the left-hand side of (22). In our case this method is especially simple and it consists of producing a sequence of $2t$-dimensional random vectors $x^{(i)}$ with normal distribution $N(0, \Lambda)$ and calculating $\sum_i (x_j^{(i)})_2 / \|x^{(i)}\|_2$, $j = 1, \ldots, 2t$, where $x^{(i)} = (x_1^{(i)}, \ldots, x_{2t}^{(i)})$.

A serious drawback of Monte Carlo method is its slow convergence which is of the order $O(n^{-1/2})$.

There also exist so-called quasi-Monte Carlo methods of integration. They need significantly less iterations, but the computation of quasi-random vectors is much more involved.

Note that Z can be seen as the function of the matrix K. Also, the matrices Z and K have the same number of zero eigenvalues.

Example 1. *If we take* $\lambda_i = i$*,* $i = 1, \ldots, 5$ *and* $K = \mathrm{diag}(\lambda_1, \ldots, \lambda_5)$*, then we obtain* $Z = \mathrm{diag}(0.8105, 0.4258, 0.2887, 0.2183, 0.1756)$

Example 2. *Let us take* $K_1 = \mathrm{diag}(10, 9, \ldots, 2, 1, 1, \ldots, 1)$*, where the size of* K *is* 100*. The Monte-Carlo integration with* 10^6 *iterations produces* $Z = \mathrm{diag}(\beta_1, \ldots, \beta_{100})$*, where* $\beta_1 = 0.068770$*,* $\beta_2 = 0.062182$*,* $\beta_3 = 0.055647$*,* $\beta_4 = 0.048532$*,* $\beta_5 = 0.041262$*,* $\beta_6 = 0.034278$*,* $\beta_7 = 0.027652$*,* $\beta_8 = 0.020550$*,* $\beta_9 = 0.013740$*,* $\beta_{10} = \cdots = \beta_{100} = 0.006900$*.*

References

[1] H. Federer, *Geometric measure theory*, Springer-Verlag, New York, 1969.

[2] W. Feller, *An introduction to probability theory and its applications, Vol. II*, John Wiley & Sons Inc., New York, 1966.

[3] J. E. Taylor, *A gaussian kinematic formula*, Ann. Probab. **34**(2006), 122–158.

[4] K. Yoshida, *Functional analysis, Classics in mathematics*, Springer-Verlag, London, 1980.