

Revisiting the Evaluation of a Multidimensional Gaussian Integral

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Abstract

The evaluation of Gaussian functional integrals is essential on the application to statistical physics and the general calculation of path integrals of stochastic processes. In this work, we present an elementary extension of an usual result of the literature as well as an alternative new derivation.

Keywords

Gaussian Integral, Determinants, Spectral Theorem, Sylvester's Criterion

1. Introduction

http://creativecommons.org/licenses/by/4.0/ In the present work, we apply theorems of Linear Algebra to derive and extend

an usual result of the literature on evaluation of multidimensional Gaussian integrals of the form [1]:

$$\int_{-\infty}^{\infty} e^{-x^{\mathrm{T}}Ax} \mathrm{d}x_{1} \cdots \mathrm{d}x_{n}$$

where \mathbf{x}^{T} is the transpose of every non-zero column vector $\mathbf{x} \in IR^{n}$ and $\mathbf{x}^{\mathrm{T}} A \mathbf{x}$ is a real positive definite quadratic form of *n* variables. In order to guarantee the convergence of the integrals, we should have

$$\boldsymbol{\varepsilon}^{\mathrm{T}} \boldsymbol{A} \boldsymbol{x} > 0 \tag{1}$$

We can also write A as a sum of its symmetric and skew-symmetric com-

ponents,
$$A = \left(\frac{A + A^{\mathrm{T}}}{2}\right) + \left(\frac{A - A^{\mathrm{T}}}{2}\right)$$
 and we have
 $\mathbf{x}^{\mathrm{T}} A \mathbf{x} = \mathbf{x}^{\mathrm{T}} \left(\frac{A + A^{\mathrm{T}}}{2}\right) \mathbf{x} > 0$ (2)

since
$$\mathbf{x}^{\mathrm{T}}\left(\frac{\mathbf{A}-\mathbf{A}^{\mathrm{T}}}{2}\right)\mathbf{x} \equiv 0$$

2. Application of the Spectral Theorem of Linear Algebra

From the Spectral Theorem of Linear Algebra [2], a real matrix will be diagonalized by an orthogonal transformation if and only if this matrix is symmetric.

We then apply an orthogonal transformation to the quadratic form

$$\mathbf{x}^{\mathrm{T}} \left(\frac{A + A^{\mathrm{T}}}{2} \right) \mathbf{x} :$$
$$\mathbf{x} = \theta \mathbf{y}; \ \mathbf{x}^{\mathrm{T}} = \mathbf{y}^{\mathrm{T}} \theta^{\mathrm{T}}; \ \theta^{\mathrm{T}} \theta = \mathbf{l} \mathbf{l}$$
(3)

where the columns of the matrix θ are the orthonormal eigenvectors of the

matrix
$$\left(\frac{A+A^2}{2}\right)$$
.

We then have

$$\theta^{\mathrm{T}}\left(\frac{A+A^{\mathrm{T}}}{2}\right)\theta = \left(\frac{A+A^{\mathrm{T}}}{2}\right)_{d}$$
(4)

where $\left(\frac{A+A^{T}}{2}\right)_{d}$ is the corresponding diagonal form.

From Equation (3) and Equation (4) we have:

$$\det\left(\frac{A+A^{\mathrm{T}}}{2}\right) = \det\left(\frac{A+A^{\mathrm{T}}}{2}\right)_{d} = \lambda_{1}^{n_{1}}\lambda_{2}^{n_{2}}\cdots\lambda_{l}^{n_{l}}$$
(5)

where $\lambda_1, \dots, \lambda_l$ are the eigenvalues and n_1, \dots, n_l their algebraic multiplicities [2] with

$$n_1 + n_2 + \dots + n_l = n \tag{6}$$

The transformation of the volume element is

$$dx_1 \cdots dx_n = \det \theta dy_1 \cdots dy_n \tag{7}$$

and we can choose

$$\det \theta = 1 \tag{8}$$

from Equation (3) and the adequate organization of the orthonormal eigenvectors as the columns of the matrix θ .

The quadratic form can then be written as

$$\boldsymbol{x}^{\mathrm{T}} A \boldsymbol{x} = \boldsymbol{y}^{\mathrm{T}} \left(\frac{A + A^{\mathrm{T}}}{2} \right)_{d} \boldsymbol{y}$$

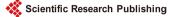
= $\lambda_{1} \sum_{j=1}^{n_{1}} y_{j}^{2} + \dots + \lambda_{l} \sum_{j=n-n_{l}+1}^{n} y_{j}^{2}$ (9)

From Equation (8) and Equation (9), the multidimensional integral will result

$$\int_{-\infty}^{\infty} e^{-x^{\mathrm{T}}Ax} \mathrm{d}x_{1} \cdots \mathrm{d}x_{n} = \int_{-\infty}^{\infty} e^{-y^{\mathrm{T}} \left(\frac{A+A^{\mathrm{T}}}{2}\right)_{d}^{y}} \mathrm{d}y_{1} \cdots \mathrm{d}y_{n}$$

$$= \prod_{j=1}^{n_{1}} \int_{-\infty}^{\infty} e^{-\lambda_{1}y_{j}^{2}} \mathrm{d}y_{j} \cdots \prod_{j=n-n_{l}+1}^{n} \int_{-\infty}^{\infty} e^{-\lambda_{l}y_{j}^{2}} \mathrm{d}y_{j}$$
(10)

since each unidimensional integral is given by



$$\int_{-\infty}^{\infty} e^{-\lambda_k y_j^2} \mathrm{d}y_j = \left(\frac{\pi}{\lambda_k}\right)^{1/2}, \quad k = 1, \cdots, l.$$
(11)

We finally write, from Equations ((5), (10), (11)),

$$\int_{-\infty}^{\infty} e^{-x^{\mathrm{T}}Ax} \mathrm{d}x_{1} \cdots \mathrm{d}x_{n} = \left(\frac{\pi^{n}}{\lambda_{1}^{n_{1}} \lambda_{2}^{n_{2}} \cdots \lambda_{l}^{n_{l}}}\right)^{1/2} = \left(\frac{\pi^{n}}{\det\left(\frac{A+A^{\mathrm{T}}}{2}\right)}\right)^{1/2}$$
(12)

and we see from Equation (12) that the original matrix A does not need to be diagonalizable [1]. The usual result of the literature will follows if $A = A^{T}$, i.e., if A is itself a symmetric matrix.

3. Application of Sylvester's Criterion Theorem

We now present an alternative derivation of the result obtained above. We will show that there is no need to apply an orthogonal transformation to diagonalize a quadratic form in order to derive formula (12).

Let us write the IR^n vectors:

$$\mathbf{x} = \sum_{j=1}^{n} x_j \hat{e}_j, \quad \mathbf{b}_j = \sum_{k=1}^{n} b_{jk} \hat{e}_k$$
 (13)

where \hat{e}_{i} , $j = 1, \dots, n$ is an orthonormal basis,

$$\hat{e}_j \cdot \hat{e}_k = \delta_{jk} \tag{14}$$

We now define the matrices

$$B_{j\times j} = \begin{pmatrix} \boldsymbol{b}_1 \cdot \hat{\boldsymbol{e}}_1 & \cdots & \boldsymbol{b}_1 \cdot \hat{\boldsymbol{e}}_{j-1} & \boldsymbol{b}_1 \cdot \hat{\boldsymbol{e}}_j \\ \vdots & \ddots & \vdots & \vdots \\ \boldsymbol{b}_j \cdot \hat{\boldsymbol{e}}_1 & \cdots & \boldsymbol{b}_j \cdot \hat{\boldsymbol{e}}_{j-1} & \boldsymbol{b}_j \cdot \hat{\boldsymbol{e}}_j \end{pmatrix} = \begin{pmatrix} b_{11} & \cdots & b_{1j-1} & b_{1j} \\ \vdots & \ddots & \vdots & \vdots \\ b_{j1} & \cdots & b_{jj-1} & b_{jj} \end{pmatrix}$$
(15)

$$B_{x}_{j\times j} = \begin{pmatrix} \boldsymbol{b}_{1} \cdot \hat{\boldsymbol{e}}_{1} & \cdots & \boldsymbol{b}_{1} \cdot \hat{\boldsymbol{e}}_{j-1} & \boldsymbol{b}_{1} \cdot x \\ \vdots & \ddots & \vdots & \vdots \\ \boldsymbol{b}_{j} \cdot \hat{\boldsymbol{e}}_{1} & \cdots & \boldsymbol{b}_{j} \cdot \hat{\boldsymbol{e}}_{j-1} & \boldsymbol{b}_{j} \cdot x \end{pmatrix} = \begin{pmatrix} b_{11} & \cdots & b_{1j-1} & \boldsymbol{b}_{1} \cdot x \\ \vdots & \ddots & \vdots & \vdots \\ b_{j1} & \cdots & b_{jj-1} & \boldsymbol{b}_{j} \cdot x \end{pmatrix}$$
(16)

The first (j-1) terms of the expansion of x will produce null determinants of the B_x matrix. The j^{th} term will correspond to the determinant det $B_{j\times j}$ times x_j . The $(j+1)^{th}$ term will lead to a determinant of a B_{j+1} matrix which is obtained by replacement of j^{th} column of the matrix $B_{j\times j}$ by a column whose elements are $b_{1j+1} \cdots b_{jj+1}$, times x_{j+1} . The n^{th} term will correspond to the determinant of a B_n matrix which is obtained by replacement of j^{th} column of the matrix $B_{j\times j}$ by a column of the matrix $B_{j\times j}$ by a column of the matrix $B_{j\times j}^{j\times j}$ by a column whose elements are $b_{1j+1} \cdots b_{jj+1}$, times x_{j+1} . The n^{th} term will correspond to the determinant of a B_n matrix which is obtained by replacement of the j^{th} column of the matrix $B_{j\times j}^{j\times j}$ by a column whose elements are $b_{1n} \cdots b_{in}$, times x_n . We can then write,

$$\det B_{x_{j\times j}} = x_j \det B_{j\times j} + \sum_{k=j+1}^n x_k \det B_{k_{j\times j}}$$
(17)

It should be noted that if $B_{n \times n} = B$ is a symmetric matrix like $B = \frac{A + A^{T}}{2}, \forall A$,

the quadratic form $\mathbf{x}^{\mathrm{T}} B \mathbf{x}$ can be written as

$$\boldsymbol{x}^{\mathrm{T}} \boldsymbol{A} \boldsymbol{x} \equiv \boldsymbol{x}^{\mathrm{T}} \boldsymbol{B} \boldsymbol{x} = \sum_{j=1}^{n} \frac{\left(\det \boldsymbol{B}_{\boldsymbol{x}}\right)^{2}}{\det \boldsymbol{B}_{j-1\times j-1} \det \boldsymbol{B}_{j\times j}}$$
(18)

where

det
$$B_{0\times 0} = 1$$
, det $B_{1\times 1} = b_{11}$, det $B_{x}_{1\times 1} = \boldsymbol{b}_{1} \cdot \boldsymbol{x}$

From Equation (17), we can write Equation (18) as

$$\boldsymbol{x}^{\mathrm{T}} A \boldsymbol{x} = \sum_{j=1}^{n} \frac{\det B_{j \times j}}{\det B_{j-1 \times j-1}} \left(x_{j} + \frac{1}{\det B_{j \times j}} \sum_{k=j+1}^{n} x_{k} \det B_{k} \right)^{2}$$
(19)

From Sylvester's Criterion [3], the quadratic form $\mathbf{x}^{\mathrm{T}} B \mathbf{x}$ is positive definite if and only if all upper left determinants $(\det B_{j \times j}, j = 1, \dots, n)$ of the symmetric matrix \mathbf{B} are positive. We should note [4] that for each variable x_j :

$$\int_{-\infty}^{\infty} e^{-\frac{\det B_{j\times j}}{\det B_{j-l\times j-l}} \left(x_j + \frac{1}{\det B_{j\times j}} \sum_{k=j+1}^n x_k \det B_k\right)^2} dx_j = \left(\frac{\pi}{\frac{\det B_{j\times j}}{\det B_{j-l\times j-l}}}\right)^{\frac{1}{2}}$$
(20)

since the other variables x_{j+1}, \dots, x_n which are contained on the term

 $\frac{1}{\det B_{j\times j}} \sum_{k=j+1}^{n} x_k \det B_k_{j\times j}$ do not contribute to unidimensional integrals of the form

$$\int_{-\infty}^{\infty} e^{-\alpha \left(x_j + f\left(x_{j+1}, \cdots, x_n\right)\right)^2} \mathrm{d}x_j = \left(\frac{\pi}{\alpha}\right)^{1/2}$$

where α is a real constant and f a generic function of its arguments.

We then have from Equation (19) and Equation (20):

$$\int_{-\infty}^{\infty} e^{-x^{\mathrm{T}}Ax} \mathrm{d}x_{1} \cdots \mathrm{d}x_{n} = \prod_{j=1}^{n} \left(\frac{\pi}{\frac{\mathrm{det} B_{j \times j}}{\mathrm{det} B_{j-1 \times j-1}}} \right)^{1/2} = \left(\frac{\pi^{n}}{\mathrm{det} B} \right)^{1/2}$$

$$= \left(\frac{\pi^{n}}{\mathrm{det} \left(\frac{A+A^{\mathrm{T}}}{2} \right)} \right)^{1/2} q.e.d.$$
(21)

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