THE MULTIVATIATE
GAUSSIAN INTEGRAL

SUBJECT

MATHEMATICS

BY

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1 Introduction - the n-dimensional Gaussian integral

The problem to solve in this tutorial is to compute the n-dimensional Gaussian integral defined as. The n-dimensional Gaussian integral has applications in quantum field theory and it's very beautiful to calculate as it combines a lot of linear algebra and multivariable calculus.

ref https://link.springer.com/chapter/10.1007/978-1-4612-12

Before introducing the integral, it is necessary to remember the definition of a positive definite matrix.

Definition 1.1 (positive definite matrix). *Let $\mathbf{A}$ be a $n \times n$ symmetric real matrix. $\mathbf{A}$ is positive definite iff $\boldsymbol{x}^\top \mathbf{A}\boldsymbol{x} > 0 \ \forall \boldsymbol{x} \in \mathbb{R}^n - \mathbf{0}$. Equivalently, $\mathbf{A}$ is positive definite iff all its eigenvalues $\lambda_1, \ldots, \lambda_n$ are strictly positive.*

Proof that these statements are equivalent is obtained by diagonalising matrix $\mathbf{A}$.

Definition 1.2 (n-dim. Gaussian integral). *Given a real symmetric and positive-definite matrix $\mathbf{A}$ of $n \times n$, it is defined as*

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\ldots\int_{-\infty}^{\infty} \exp(-\boldsymbol{x}^\top \mathbf{A}\boldsymbol{x})\, dx_1\, dx_2 \ldots dx_n \tag{1.1}$$

Before attempting to compute it, two techniques are required.

1. How to compute 1D Gaussian integrals.
2. How to perform change of variables in a multivariate integral.

1.1 Requirements

1.1.1 1D Gaussian integral

Corollary 1.1 (Gaussian integral).

$$\int_{-\infty}^{\infty} \exp(-\alpha x^2) = \sqrt{\frac{\pi}{\alpha}} \tag{1.2}$$

Proof. We start by proving a simpler result for $\alpha = 1$; that

$$I := \int_{-\infty}^{\infty} \exp(-x^2)\, dx = \sqrt{\pi}$$

Changing (renaming) the dummy variable x to y:

$$I = \int_{-\infty}^{\infty} \exp(-y^2)\, dy$$

$$\therefore I^2 = \int_{-\infty}^{\infty} \exp(-y^2)\, dy \int_{-\infty}^{\infty} \exp(-x^2)\, dx = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \exp(-x^2 - y^2)\, dx dy$$

If we change from Cartesian to polar coordinates in I^2, i.e. $x := \cos(\theta)$, $y := \sin(\theta)$, then $x^2 + y^2 = r^2$ and $dxdy = rdrd\theta$ [1]. The Cartesian integral limits cover the entire xy plane and so much the polar limits for r, θ. Therefore r ranges from 0 to ∞ and θ from 0 to 2π.

$$\therefore I^2 = \int_0^{2\pi}\int_0^{\infty} \exp(-r^2) r dr d\theta$$

Letting $u := -r^2 \Rightarrow rdr = -u/2$, the limits change $r = 0 \Rightarrow u \to \infty$, $r \to \infty \Rightarrow u \to -\infty$ and the integral becomes

$$I^2 = -\frac{1}{2}\int_0^{2\pi}\int_0^{-\infty} \exp(u)\, du d\theta = -\frac{1}{2}\int_0^{2\pi} -d\theta = \pi$$

To conclude,

$$I = \int_{-\infty}^{\infty} \exp(-x^2)\, dx = \sqrt{\pi}$$

Finally, substituting in I $x := \sqrt{\alpha} y$, $\alpha > 0$, then $dx = \sqrt{\alpha} dy$, therefore

$$\int_{-\infty}^{\infty} \exp(-\alpha y^2)\sqrt{\alpha} dy = \sqrt{\pi} \Rightarrow$$

$$\int_{-\infty}^{\infty} \exp(-\alpha y^2) dy = \sqrt{\frac{\pi}{\alpha}}$$

[1] Proof for $dxdy = rdrd\theta$ in A.1

□

1.1.2 Change of variables in a multivariable integral

Before introducing the change of variables the change of variables, it is necessary to introduce a scalar quantity called Jacobian

Definition 1.3 (Jacobian). *For a transformation $\Phi\ \mathbb{R}^m \to \mathbb{R}^n : (x_1, \ldots, x_m) \to \big(f_1(x_1, \ldots, x_n), \ldots, f_n(x_m)\big)$, the Jacobian is defined as the determinant*

$$J = \det\left(\begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & \cdots & \frac{\partial f_1}{\partial x_m} \\ \frac{\partial f_2}{\partial x_2} & \frac{\partial f_2}{\partial x_2} & \cdots & \frac{\partial f_2}{\partial x_m} \\ \ldots & \ldots & \ddots & \vdots \\ \frac{\partial f_n}{\partial x_2} & \frac{\partial f_n}{\partial x_2} & \cdots & \frac{\partial f_n}{\partial x_m} \end{bmatrix}\right)$$

The matrix of partial derivatives in the determinant is called Jacobian matrix. The latter matrix is often denoted as $\frac{\partial(f_1, \ldots, f_n)}{\partial(x_1, \ldots, x_m)}$ or ∇f for shorthand.

Example 1.1. *Compute the Jacobian of the transformation from Cartesian to polar coordinates $\Phi : (x, y) \to (r, \theta)$ defined as $x = r\cos(\theta),\ \ y = r\sin(\theta)$.*

Solution 1.1.

$$J = \det\left(\begin{bmatrix} \frac{\partial x}{\partial r} & \frac{\partial x}{\partial \theta} \\ \frac{\partial y}{\partial r} & \frac{\partial y}{\partial \theta} \end{bmatrix}\right)$$

Compute partial derivatives

$$\frac{\partial x}{\partial r} = \cos\theta, \qquad \frac{\partial x}{\partial \theta} = -r\sin\theta$$

$$\frac{\partial y}{\partial r} = \sin\theta, \qquad \frac{\partial y}{\partial \theta} = r\cos\theta$$

Substitute

$$\therefore J = \det\left(\begin{bmatrix} \cos\theta & -r\sin\theta \\ \sin\theta & r\cos\theta \end{bmatrix}\right) = r$$

Lemma 1.1 (Change of variables). *If an "1-1" mapping $\Phi : (x, y) \to \big(u(x, y), v(x, y)\big)$ sends a region D in xy-space to a region D^* in uv-space, then*

$$\int\int_D f(x, y)\,dx\,dy = \int\int_{D^*} f(u(x, y), v(x, y)) \left|\frac{\partial(u, v)}{\partial(x, y)}\right| du\,dv \tag{1.3}$$

Notes:

1. Obviously this definition can be generalised in n-dimensional mappings but is stated in 2D for clarity.
2. $|.|$ denotes absolute value – we need the absolute Jacobian!
3. The proof of Lemma 1.1 in n dimensions is omitted but a neat proof is found in .

ref: https://math.stackexchan
com/questions/267267/intuitive-p

2 Computing the integral

To reiterate, the integral to compute is the following

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty} \exp(-\mathbf{x}^\top \mathbf{A}\mathbf{x})\,dx_1\,dx_2 \ldots dx_n$$

For succinctness, we denote as D the integration space, which is a subspace of $\mathbb{R}^n$, and the integral as

$$\int_D \exp(-\mathbf{x}^\top \mathbf{A}\mathbf{x})\,dx_1\,dx_2 \ldots dx_n$$

Because $\mathbf{A}$ is symmetric and real, it's diagonalisable, which means that there exists an orthonormal (therefore symmetric as well) matrix $\mathbf{S}$ such that

$$\mathbf{S}^{-1}\mathbf{A}\mathbf{S} = \mathbf{D}, \quad \mathbf{D} = \begin{bmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_n \end{bmatrix}, \quad \lambda_1 > \ldots > \lambda_n > 0 \tag{1}$$

Positive eigenvalues λ_i are guaranteed as $\mathbf{A}$ is positive definite. Because $\mathbf{S}$ is orthonormal, $\mathbf{S}^{-1} = \mathbf{S}^\top$, therefore Eq. (1) can be rewritten as

$$\mathbf{S}^\top\mathbf{A}\mathbf{S} = \mathbf{D} \Rightarrow \mathbf{A} = \mathbf{S}\mathbf{D}\mathbf{S}^\top \tag{2}$$

The integral is hence rewritten

$$I = \int_D \exp(-\mathbf{x}^\top\mathbf{S}\mathbf{D}\mathbf{S}^\top\mathbf{x})\, dx_1\, dx_2 \ldots dx_n \tag{3}$$

Substitute $\mathbf{y} = \mathbf{S}^\top\mathbf{x}$, therefore $\mathbf{y}^\top = \mathbf{x}^\top\mathbf{S}$. The differentials $dx_1, \ldots, dx_n$ will be transformed to $|J|\, dy_1, \ldots, dy_n$ as stated in Lemma 1.1, where J is the Jacobian of the linear transform $f(\mathbf{x}) = \mathbf{S}^\top\mathbf{x}$. As proven in A.3, $J = \det(S^\top)$. As proven in turn in A.2, the determinant of an orthogonal matrix such as $\mathbf{S}^\top$ is 1. Therefore the new differentials are simply

$$dy_1 \ldots dy_n = dx_1 \ldots dx_n \tag{4}$$

Integral I is therefore transformed to

$$I = \int_D \exp(-\mathbf{y}^\top\mathbf{D}\mathbf{y})\; dy_1 \ldots dy_n \tag{5}$$

The scalar quantity $\mathbf{y}^\top\mathbf{D}\mathbf{y}$ is called quadratic form of $\mathbf{D}$ and because the latter is diagonal as defined in Eq. (1), it's easy to see that it equals

$$\mathbf{y}^\top\mathbf{D}\mathbf{y} = \lambda_1 y_1^2 + \ldots + \lambda_n y_n^2 \tag{6}$$

Substituting Eq. (6) in Eq. (5), the integral is simplified to

$$I = \int_D \exp(-\lambda_1 y_1^2 - \ldots - \lambda_n y_n^2) dy_1 \ldots dy_n \tag{7}$$

Expanding the integral the 1-dimensional real subspaces of $\mathbb{R}^n$ (since D is in $\mathbb{R}^n$) and breaking the exponential, it can be rewritten as

$$I = \int_{D_1} \exp(-\lambda_1 y_1^2) dy_1 \ldots \int_{D_n} \exp(-\lambda_n y_n^2) dy_n \tag{8}$$

Now each one can be calculated individually. Each sub-integral is a Gaussian one with $\alpha = \lambda_i$, therefore from Eq. (1.2)

$$\int_{D_i} \exp(-\lambda_i y_i^2) dy_i = \sqrt{\frac{\pi}{\lambda_i}}, \quad i = 1, \ldots, n \tag{9}$$

Finally, from Eq. (8) given Eq. (9)

$$\int_{D_1} \exp(-\lambda_1 y_1^2) dy_1 \ldots \int_{D_n} \exp(-\lambda_n y_n^2) dy_n = \sqrt{\frac{\pi^n}{\lambda_1 \ldots \lambda_n}} \tag{10}$$

Note that the product $\lambda_1 \ldots \lambda_n$ is simply the determinant of the diagonal matrix $\mathbf{D}$ from Eq. (1), which contains the eigenvalues of $\mathbf{A}$. Therefore $\lambda_1 \ldots \lambda_n = \det(\mathbf{D})$. Thus the final result is obtained.

COROLLARY 2.1 ($n - dimensionalGaussianintegral$)**.**

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \ldots \int_{-\infty}^{\infty} \exp(-\boldsymbol{x}^\top\boldsymbol{A}\boldsymbol{x})\, dx_1\, dx_2 \ldots dx_n = \sqrt{\frac{\pi^n}{\det(\boldsymbol{D})}} \tag{2.1}$$

A Appendices

A.1 Lemma proof; Cartesian to polar differentials and $r\,dr\,d\theta$

Lemma A.1. *If we transform from Cartesian to polar coordinates in the integral $I = \int\int_Q f(x,y)\,dx\,dy$ over some area Q by setting $x = r\cos(\theta)$, $y = r\,cos(\theta)$, then:*

$$\int\int_Q f(x,y)\,dx\,dy = \int\int_A f(r\cos(\theta), r\sin(\theta))\,r\,dr\,d\theta \tag{A.1}$$

Proof. Suppose we evaluate the integral over a polar region defined by $\alpha \leq \theta \leq \beta$, $g(\theta) \leq r \leq f(\theta)$, where the curves $f(\theta), g(\theta)$ are contained between two radii $p, q, \quad p < q$. We infinitesimally partition θ in $\theta_0, \dots, \theta_m$ and r in $r_0, \dots, r_n$ (Fig. 1).

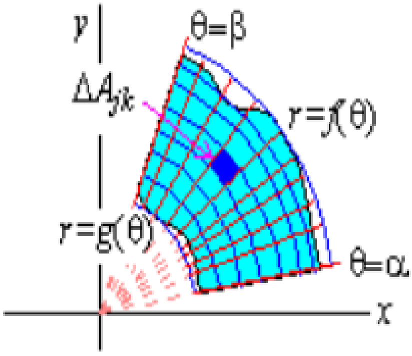

Fig. 1. Expressing the area as the union of infinitesimal polar partitions.

Then the area dA of each tiny wedge is simply (Fig. 2) the difference between the sector from 0 to $r + dr$ minus the sector from 0 to r:

$$\begin{aligned} dA &= \frac{1}{2}(r + dr)^2 d\theta - \frac{1}{2} r^2 d\theta \\ &= \frac{2r + dr}{2} dr\,d\theta \\ &= r^* dr\,d\theta \end{aligned}$$

, where $r^* := \frac{2r+dr}{2}$ is the average radius of the infinitesimal wedge.

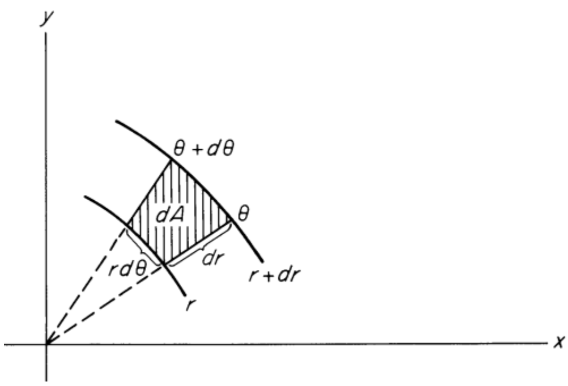

Fig. 2. Computing dA w.r.t. dr, $d\theta$.

□

In general, for the wedge jk, its area is:

$$\Delta A_{jk} \approx r_j \Delta r_j \Delta \theta_j$$

If we transform x and y in the polar domain as $x_{jk} = r_j \cos(\theta_k)$, $y_{jk} = r_j \sin(\theta_k)$, then the total area expressed by the integral is:

$$\int \int_Q f(x,y)dA = \int \int_Q f(x,y)dxdy \approx$$

$$\sum_{j=1}^{m} \sum_{i=1}^{n} f(r_i, \theta_j)\Delta A_{ij}$$

Taking the limit as $m, n \to \infty$:

$$\int \int_Q f(x,y)dA = \int_{\alpha}^{\beta} \int_{g(\theta)}^{f(\theta)} f(r,\theta) r dr d\theta$$

A.2 Lemma proof; determinant of orthogonal matrix is ± 1

LEMMA A.2. *The determinant of an orthogonal matrix is* ± 1.

Proof. Let $\mathbf{U} \in \mathbb{R}^{m \times n}$ be an orthogonal matrix. The columns of an orthogonal matrix are orthonormal, which means

$$\mathbf{u}_i^\top \mathbf{u}_j = \begin{cases} 1, & i = j \\ 0, & i \neq j \end{cases}$$

for any two columns $\mathbf{u}_i, \mathbf{u}_j$. Therefore

$$\mathbf{U}^\top \mathbf{U} = \mathbf{I}_m$$

Taking determinant and using their properties:

$$\det(\mathbf{U})\det(\mathbf{U}^\top) = \det(\mathbf{I}) \Rightarrow$$

$$\det(\mathbf{U})^2 = 1 \Rightarrow$$

$$\det(\mathbf{U}) = \pm 1$$

□

A.3 Proof; Jacobian of linear transform

LEMMA A.3. *Let $\boldsymbol{X} \in \mathbb{R}^n$ and $\boldsymbol{Y} \in \mathbb{R}^n$ be two real column vectors. Let also each element of $\boldsymbol{X}$ be functionally independent (no element in $\boldsymbol{X}$ if a function of element in $\boldsymbol{Y}$ and vice versa). If $\boldsymbol{Y}$ is given by the linear transform*

$$\boldsymbol{Y} = \boldsymbol{A}\boldsymbol{X}, \quad \det(\boldsymbol{A}) \neq 0$$

, where $\boldsymbol{A} = (\alpha_{ij})$ is non-singular $p \times p$ matrix of constants, then

$$\boldsymbol{Y} = \boldsymbol{A}\boldsymbol{X}, \quad \det(\boldsymbol{A}) \neq 0 \Rightarrow d\boldsymbol{Y} = \det(\boldsymbol{A})\, d\boldsymbol{X} \tag{A.2}$$

Proof. We know that when we do change of variables with from $\mathbf{X}$ to $\mathbf{Y} = f(\mathbf{X})$, then the differentials are given by:

$$d\mathbf{Y} = \det(\mathbf{J})\, d\mathbf{X} \tag{1}$$

where $\mathbf{J}$ is the Jacobian matrix of $\mathbf{Y}$. For the linear transform $\mathbf{Y} = \mathbf{A}\mathbf{X}$, because $\mathbf{X}$ and $\mathbf{Y}$ both have length n, the Jacobian is given by:

$$\mathbf{J} = \begin{bmatrix} \frac{\partial \mathbf{Y}}{\partial x_1} & \frac{\partial \mathbf{Y}}{\partial x_2} & \cdots & \frac{\partial \mathbf{Y}}{\partial x_n} \end{bmatrix} = \begin{bmatrix} \frac{\partial \mathbf{Y}_1}{\partial x_1} & \frac{\partial \mathbf{Y}_1}{\partial x_2} & \cdots & \frac{\partial \mathbf{Y}_1}{\partial x_n} \\ \frac{\partial \mathbf{Y}_2}{\partial x_1} & \frac{\partial \mathbf{Y}_2}{\partial x_2} & \cdots & \frac{\partial \mathbf{Y}_2}{\partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial \mathbf{Y}_n}{\partial x_1} & \frac{\partial \mathbf{Y}_n}{\partial x_2} & \cdots & \frac{\partial \mathbf{Y}_n}{\partial x_n} \end{bmatrix} \tag{2}$$

However, each element y_i of $\mathbf{Y}$ is given by:

$$y_i = \alpha_{i1}x_1 + \alpha_{i2}x_2 + \ldots + \alpha_{in}x_n, \quad i = 1, \ldots, n$$

Therefore each entry (i, j) of the Jacobian is given by:

$$\frac{\partial y_i}{\partial x_j} = \alpha_{ij} \quad \forall\, i = 1, \ldots, n, \quad \forall\, j = 1, \ldots, n \tag{3}$$

i.e. $\mathbf{J} = \mathbf{A}$. Therefore Eq. (1) with the aid of Eq. (2), Eq. (3) yields:

$$d\mathbf{Y} = \det(\mathbf{A})\, d\mathbf{X}$$

□