

Error integral

Multidimensional Gauss error function

Christophe De Beule (christophe.debeule@gmail.com)

Consider the following integral:

$$I_N^{(k)}(A, t) = \prod_{i \neq k}^N \int_{-\infty}^{\infty} dx_i \int_{-t}^t dx_k e^{-\mathbf{x}^\top A \mathbf{x}},$$

where A is a positive definite real symmetric N -dimensional matrix, $t > 0$, and $N > 0$ is an integer. For $N = 1$, with $d = A > 0$, the integral becomes

$$I_1(A, t) = \sqrt{\frac{\pi}{d}} \operatorname{erf}(t\sqrt{d}).$$

Next, we consider the case $N > 1$. First, we transform to new coordinates \mathbf{y} by diagonalizing A :

$$A = B^\top D B, \quad \mathbf{y} = B \mathbf{x},$$

where D is a diagonal matrix with the eigenvalues of A which are guaranteed to be positive, and where the rows of the orthogonal matrix B are the corresponding eigenvectors. Note that this transformation has unit Jacobian, $|\det B| = 1$. The integral becomes

$$\prod_{i=1}^{N-1} \int_{-\infty}^{\infty} dy_i e^{-d_i y_i^2} \int_{y_N^a}^{y_N^b} dy_N e^{-d_N y_N^2},$$

where d_i are the elements of D , i.e. the eigenvalues of A . Because $\mathbf{x} = B^\top \mathbf{y}$, we have

$$x_k = \sum_{i=1}^N b_{ik} y_i \quad \Rightarrow \quad y_N = \frac{1}{b_{Nk}} \left(x_k - \sum_{i=1}^{N-1} b_{ik} y_i \right).$$

where b_{ik} is the element of the matrix B at row i and column k . The bounds of the integrals over y_N are therefore given by

$$y_N^a = \sum_{i=1}^{N-1} \alpha_i y_i - \beta t, \quad y_N^b = \sum_{i=1}^{N-1} \alpha_i y_i + \beta t,$$

with

$$\alpha_i = -\frac{b_{ik}}{b_{Nk}}, \quad \beta = \frac{1}{|b_{Nk}|},$$

The integral over y_N then becomes

$$\sqrt{\frac{\pi}{4d_N}} \prod_{i=1}^{N-1} \int_{-\infty}^{\infty} dy_i e^{-d_i y_i^2} \left[\operatorname{erf} \left(\sqrt{d_N} y_N^b \right) - \operatorname{erf} \left(\sqrt{d_N} y_N^a \right) \right]. \quad (1)$$

To solve the remaining integrals, we use the following result (see Appendix)

$$\int_{-\infty}^{\infty} dy e^{-dy^2} \operatorname{erf}(ay + b) = \sqrt{\frac{\pi}{d}} \operatorname{erf} \left(\frac{b}{\sqrt{1 + a^2/d}} \right). \quad (2)$$

We solve the total integral by solving the integral over y_1 first, then y_2 , and so on, until y_{N-1} . The corresponding parameters for the integral over y_1 , y_2 , and y_3 are given by

$$\begin{aligned} a_1 &= \alpha_1 \sqrt{d_N}, & b_1 &= \sqrt{d_N} \left(\sum_{i=2}^{N-1} \alpha_i y_i + \beta x_k \right), \\ a_2 &= \alpha_2 \sqrt{\frac{d_N}{1 + a_1^2/d_1}}, & b_2 &= \sqrt{\frac{d_N}{1 + a_1^2/d_1}} \left(\sum_{i=3}^{N-1} \alpha_i y_i + \beta x_k \right), \\ a_3 &= \alpha_3 \sqrt{\frac{d_N}{(1 + a_1^2/d_1)(1 + a_2^2/d_2)}}, & b_3 &= \sqrt{\frac{d_N}{(1 + a_1^2/d_1)(1 + a_2^2/d_2)}} \left(\sum_{i=4}^{N-1} \alpha_i y_i + \beta x_k \right), \end{aligned}$$

where $x_k = \pm t$ for the first and second part in (1), restrictively. The a_j can be simplified by nothing that

$$\begin{aligned} \prod_{i=1}^{j-1} \left(1 + \frac{a_i^2}{d_i} \right) &= \prod_{i=1}^{j-2} \left(1 + \frac{a_i^2}{d_i} \right) + d_N \frac{\alpha_{j-1}^2}{d_{j-1}} \\ &= 1 + d_N \sum_{i=1}^{j-1} \frac{\alpha_i^2}{d_i}, \end{aligned} \quad (3)$$

which gives

$$a_j = \alpha_j \sqrt{\frac{d_N}{1 + d_N \sum_{i=1}^{j-1} \frac{\alpha_i^2}{d_i}}}, \quad (j = 1, \dots, N-1).$$

Furthermore, using Eq. (3), we find

$$\begin{aligned} \frac{b_{N-1}}{\sqrt{1 + a_{N-1}^2/d_{N-1}}} &= \beta x_k \sqrt{\frac{d_N}{\prod_{i=1}^{N-1} (1 + a_i^2/d_i)}} \\ &= \beta x_k \sqrt{\frac{d_N}{1 + d_N \sum_{i=1}^{N-1} \frac{\alpha_i^2}{d_i}}} = \frac{x_k}{\sqrt{\sum_{i=1}^N \frac{b_{ik}^2}{d_i}}}, \end{aligned}$$

where again $x_k = \pm t$. Finally, the integral becomes

$$I_N^{(k)}(A, t) = \sqrt{\frac{\pi^N}{\det A}} \operatorname{erf} \left(\frac{t}{\sqrt{A_{kk}^{-1}}} \right),$$

where we repeatedly used (2), $\operatorname{erf}(-x) = -\operatorname{erf}(x)$, and

$$\sum_{i=1}^N \frac{b_{ik}^2}{d_i} = [B^\top D^{-1} B]_{kk} = A_{kk}^{-1}.$$

Other integral

Here, we prove Eq. (2). Consider the following integral

$$\begin{aligned} \int_{-\infty}^{\infty} dx e^{-d(x+c)^2} \operatorname{erf}(ax+b) &= \frac{2}{\sqrt{\pi}} \int_{-\infty}^{\infty} dx e^{-d(x+c)^2} \int_0^{ax+b} dy e^{-y^2} \\ &= \frac{2}{\sqrt{\pi}} \int_{-\infty}^{\infty} dx e^{-d(x+c)^2} \int_0^1 dt (ax+b) e^{-(ax+b)^2 t^2} \\ &= \frac{2}{\sqrt{\pi}} \int_0^1 dt \int_{-\infty}^{\infty} dx (ax+b) e^{-d(x+c)^2 - (ax+b)^2 t^2}, \end{aligned}$$

where we used the definition of $\text{erf}(x)$ and the substitution $t = (ax + b)y$. The exponent is given by the negative of

$$\begin{aligned}
& d(x + c)^2 + (ax + b)^2 t^2 \\
&= x^2 (d + a^2 t^2) + 2x (dc + abt^2) + dc^2 + b^2 t^2 \\
&= (d + a^2 t^2) \left(x + \frac{dc + abt^2}{d + a^2 t^2} \right)^2 + dc^2 + b^2 t^2 - \frac{(dc + abt^2)^2}{d + a^2 t^2} \\
&= (d + a^2 t^2) \left(x + \frac{dc + abt^2}{d + a^2 t^2} \right)^2 + \frac{(dc^2 + b^2 t^2)(d + a^2 t^2) - (dc + abt^2)^2}{d + a^2 t^2} \\
&= (d + a^2 t^2) \left(x + \frac{dc + abt^2}{d + a^2 t^2} \right)^2 + \frac{d(b - ac)^2 t^2}{d + a^2 t^2}.
\end{aligned}$$

Naturally, we then perform the substitution

$$x' = x + \frac{dc + abt^2}{d + a^2 t^2},$$

so that

$$\begin{aligned}
ax + b &= ax' - a \frac{dc + abt^2}{d + a^2 t^2} + b \\
&= ax' + \frac{b(d + a^2 t^2) - a(dc + abt^2)}{d + a^2 t^2} \\
&= ax' + \frac{d(b - ac)}{d + a^2 t^2}.
\end{aligned}$$

Now we can solve the integral over x' . The odd part of the integrand gives a vanishing integral and we obtain

$$\frac{2}{\sqrt{\pi}} \int_0^1 dt \frac{d(b - ac)}{d + a^2 t^2} \sqrt{\frac{\pi}{d + a^2 t^2}} e^{-\frac{d(b - ac)^2 t^2}{d + a^2 t^2}}.$$

The final integral can be solved with the substitution

$$u = \frac{(b - ac)t}{\sqrt{1 + a^2 t^2/d}} \Rightarrow du = \frac{b - ac}{(1 + a^2 t^2/d)^{3/2}} dt,$$

and we finally obtain

$$\sqrt{\frac{\pi}{d}} \frac{2}{\sqrt{\pi}} \int_0^{\frac{b - ac}{\sqrt{1 + a^2/d}}} du e^{-u^2} = \sqrt{\frac{\pi}{d}} \text{erf} \left(\frac{b - ac}{\sqrt{1 + a^2/d}} \right).$$

Other method

Previously, we found

$$\prod_{i \neq k}^N \int_{-\infty}^{\infty} dx_i \int_{-t}^t dx_k e^{-\frac{1}{2} \mathbf{x}^\top A \mathbf{x}} = (2\pi)^{N/2} (\det A)^{-1/2} \text{erf} \left(\frac{t}{\sqrt{2A_{kk}^{-1}}} \right).$$

Note, however, that

$$\begin{aligned}
\mathbf{x}^\top A \mathbf{x} &= \mathbf{x}'^\top A' \mathbf{x}' + x_k \sum_{i \neq k}^N (A_{ki} + A_{ik}) x_i + A_{kk} x_k^2 \\
&= \mathbf{x}'^\top A' \mathbf{x}' - 2x_k \mathbf{j}^\top \mathbf{x}' + A_{kk} x_k^2,
\end{aligned}$$

with \mathbf{x}' is the $(N - 1)$ -dimensional vector formed by removing x_k from \mathbf{x} , A' is the matrix formed if the k -th row and column are removed from A , and \mathbf{j} has coefficients

$$j_i = -A_{ki}, \quad (i \neq k),$$

where we used the fact that A is symmetric. Note that any principal submatrix of A is also real symmetric and positive definite. Because

$$\prod_{i \neq k}^N \int_{-\infty}^{\infty} dx_i e^{-\frac{1}{2} \mathbf{x}'^\top A' \mathbf{x}' + x_k \mathbf{j}^\top \mathbf{x}'} = (2\pi)^{(N-1)/2} (\det A')^{-1/2} e^{\frac{1}{2} \mathbf{j}^\top A'^{-1} \mathbf{j} x_k^2},$$

the final integral becomes

$$(2\pi)^{(N-1)/2} (\det A')^{-1/2} \int_{-t}^t dx_k e^{-\frac{1}{2} (A_{kk} - \mathbf{j}^\top A'^{-1} \mathbf{j}) x_k^2}.$$

Comparing this result with our previous result, we need to prove that

$$A_{kk} - \mathbf{j}^\top A'^{-1} \mathbf{j} = \frac{1}{A_{kk}^{-1}},$$

To this end, we first note that

$$A_{kk}^{-1} = \frac{\det A'}{\det A},$$

because $\det A'$ is the cofactor of A_{kk} . Furthermore, we find

$$\begin{aligned} \mathbf{j}^\top A'^{-1} \mathbf{j} &= \sum_{i \neq k}^N A_{ki} \sum_{j \neq k}^N A_{jk} A'_{ij}{}^{-1} \\ &= \frac{1}{\det A'} \sum_{i \neq k}^N A_{ki} \sum_{j \neq k}^N A_{jk} (-1)^{i+j} M_{ji} \\ &= -\frac{1}{\det A'} \sum_{i \neq k}^N (-1)^{k+i} A_{ki} \sum_{j \neq k}^N (-1)^{j+k-1} A_{jk} M_{ji} \\ &= \frac{A_{kk} \det A' - \det A}{\det A'} = A_{kk} - \frac{1}{A_{kk}^{-1}}, \end{aligned}$$

where M_{ji} is the (j, i) minor of A' . We arrive at the same result, thusly.