Error integral

Multidimensional Gauss error function

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Consider the following integral:

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

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 $\boldsymbol{y}$ by diagonalizing A:

$$A = B^\top D B, \qquad \boldsymbol{y} = B\boldsymbol{x},$$

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 $\boldsymbol{x} = B^\top \boldsymbol{y}$, 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

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

with

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

The integral over y_N then becomes

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

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

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

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

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

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

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

which gives

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

Furthermore, using Eq. (3), we find

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

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

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

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

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

Other integral

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

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

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

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

Naturally, we then perform the substitution

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

so that

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

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

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

The final integral can be solved with the substitution

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

and we finally obtain

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

Other method

Previously, we found

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

Note, however, that

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

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

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

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

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

the final integral becomes

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

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

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

To this end, we first note that

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

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

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

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