GAUSSIAN INTEGRALS: SINGLE VARIABLE & MATRIX EXPONENTS

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References: Anthony Zee, *Quantum Field Theory in a Nutshell*, 2nd edition (Princeton University Press, 2010) - Chapter I.2, Appendix 2.

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A *Gaussian integral* has the form

$$G=\int_{-\infty}^{\infty}e^{-x^{2}}dx \tag{1}$$

There is no closed form indefinite integral (without the limits) in terms of elementary functions, but it turns out that, with the infinite limits, the integral is quite easy to using a simple trick. The trick is to square the integral and convert to polar coordinates, using $r^2=x^2+y^2$.

$$\begin{aligned}
G^{2} &= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}e^{-x^{2}-y^{2}}dxdy && (2)\\
&= \int_{0}^{\infty}\int_{0}^{2\pi}re^{-r^{2}}d\theta dr && (3)\\
&= 2\pi\int_{0}^{\infty}re^{-r^{2}}dr && (4)\\
&= \pi\left(-e^{-r^{2}}\right)\Big|_{0}^{\infty} && (5)\\
&= \pi && (6)
\end{aligned}$$

Taking the square root gives

$$G=\int_{-\infty}^{\infty}e^{-x^{2}}dx=\sqrt{\pi} \tag{7}$$

We can generalize this to the case where the exponent is a general quadratic in x, that is

$$\int_{-\infty}^{\infty}e^{-ax^{2}+bx}dx \tag{8}$$

where $a>0$ (if $a<0$ the integral diverges). The trick here is to complete the square in the quadratic:

$$
\begin{aligned}
-ax^2+bx &= -a\left(x^2-\frac{b}{a}x\right) &(9)\\
&= -a\left(x-\frac{b}{2a}\right)^2+\frac{b^2}{4a} &(10)
\end{aligned}
$$

Now use the substitution $u \equiv \sqrt{a}\left(x-\frac{b}{2a}\right)$, $du=\sqrt{a}dx$ to get

$$
\begin{aligned}
\int_{-\infty}^{\infty} e^{-ax^2+bx}dx &= \frac{1}{\sqrt{a}}e^{b^2/4a}\int_{-\infty}^{\infty} e^{-u^2}du &(11)\\
&= \sqrt{\frac{\pi}{a}}e^{b^2/4a} &(12)
\end{aligned}
$$

We can generalize this even further by considering an exponent of the form $-\frac{1}{2}x^TAx+J^Tx$, where x and J are now N-dimensional vectors and A is a real symmetric $N\times N$ matrix, with x^T being the transpose of x. With these definitions, the exponent $-x^TAx+J^Tx$ is a scalar, although it now contains N independent coordinates x_i for $i=1,\ldots,N$ rather than just the single x we've been considering so far. In this case the Gaussian integral becomes

$$
\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty}dx_1dx_2\ldots dx_N e^{-\frac{1}{2}x^TAx+J^Tx} \tag{13}
$$

To derive a formula for this integral, we need a theorem from linear algebra which states that we can decompose a real symmetric matrix A into the form

$$
A=O^{-1}DO \tag{14}
$$

where D is a diagonal matrix whose diagonal elements are the eigenvalues of A and O is an orthonormal matrix, that is a matrix with determinant 1 and such that $O^{-1}=O^T$. The matrix O is therefore a rotation matrix in N dimensional Euclidean space.

We can now make the substitution

$$
y=Ox \tag{15}
$$

which applies the rotation O to the original coordinates x. Then $x=O^{-1}y=O^Ty$ and $x^T=y^TO$, so

$$-\frac{1}{2}x^T Ax + J^T x = -\frac{1}{2}y^T O\left(O^{-1}DO\right)O^{-1}y + J^T O^T y \tag{16}$$

$$= -\frac{1}{2}y^T Dy + (OJ)^T y \tag{17}$$

Because D is diagonal, we get

$$-\frac{1}{2}y^T Dy = -\frac{1}{2}\sum_{i=1}^{N} D_{ii}y_i^2 \tag{18}$$

$$(OJ)^T y = \sum_{i=1}^{N} (OJ)_i y_i \tag{19}$$

That is, the exponential in the integral 13 has decoupled into a product of independent integrals, each of the form 8.

One final point needs to be addressed, and that's the transformation of the volume element $dx_1 dx_2 \ldots dx_N$ into the y_i coordinates. Because the x and y coordinate systems are related by a rigid rotation 15, the volume elements are the same in the two coordinate systems, so $dx_1 dx_2 \ldots dx_N$ just becomes $dy_1 dy_2 \ldots dy_N$. Therefore we get

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty} dx_1 dx_2 \ldots dx_N e^{-\frac{1}{2}x^T Ax + J^T x} = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty} dy_1 dy_2 \ldots dy_N e^{-\frac{1}{2}\sum_{i=1}^{N} D_{ii}y_i^2 + \sum_{i=1}^{N}(OJ)} \tag{20}$$

$$= \prod_{i=1}^{N}\int_{-\infty}^{\infty} dy_i e^{-\frac{1}{2}D_{ii}y_i^2 + (OJ)_i y_i} \tag{21}$$

$$= \left[\prod_{i=1}^{N}\sqrt{\frac{2\pi}{D_{ii}}}\right] e^{\sum_{i=1}^{N}(OJ)_i^2/2D_{ii}} \tag{22}$$

To simplify this result, we can fiddle with the matrices a bit. From 14

$$A^{-1} = O^{-1}D^{-1}O \tag{23}$$

The inverse of a diagonal matrix D is another diagonal matrix whose diagonal elements are $1/D_{ii}$: $\left(D^{-1}\right)_{ii} = \frac{1}{D_{ii}}$. Therefore $(OJ)^T D^{-1}(OJ)$ is $\sum_{i=1}^{N}(OJ)_i^2/D_{ii}$, and:

$$
\begin{aligned}
(OJ)^T D^{-1} (OJ) &= J^T O^T D^{-1} O J && (24)\\
&= J^T O^{-1} D^{-1} O J && (25)\\
&= J^T A^{-1} J && (26)
\end{aligned}
$$

Also, taking the determinant of 14 we get (remember $\det O = \det O^{-1} = 1$):

$$\det A = \det D = \prod_{i=1}^{N} D_{ii} \tag{27}$$

Finally we get

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\ldots\int_{-\infty}^{\infty} dx_1 dx_2 \ldots dx_N e^{-\frac{1}{2}x^T Ax + J^T x} = \sqrt{\frac{(2\pi)^N}{\det A}} e^{\frac{1}{2}J^T A^{-1} J} \tag{28}$$

Example. We can test this formula in the 2-d case using

$$
\begin{aligned}
A &= \begin{bmatrix} 6 & 2 \\ 2 & 3 \end{bmatrix} && (29)\\
A^{-1} &= \frac{1}{7}\begin{bmatrix} \frac{3}{2} & -1 \\ -1 & 3 \end{bmatrix} && (30)\\
\det A &= 14 && (31)\\
J &= \begin{bmatrix} 0.5 \\ 0.6 \end{bmatrix} && (32)\\
J^T A^{-1} J &= 0.1221 && (33)\\
\sqrt{\frac{(2\pi)^N}{\det A}} e^{\frac{1}{2}J^T A^{-1} J} &= 1.785 && (34)
\end{aligned}
$$

We can check this by evaluating the integral 13 directly (I did this using Maple). The exponent is

$$-\frac{1}{2}x^T Ax + J^T x = -3x_1^2 - 2x_1 x_2 - \frac{3}{2}x_2^2 + 0.5x_1 + 0.6x_2 \tag{35}$$

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} dx_1 dx_2 e^{-\frac{1}{2}x^T Ax + J^T x} = 1.785 \tag{36}$$

This verifies the formula 28. [If you want to do the integrals by completing the square, do the x_1 integral first by completing the square on the quadratic in x_1, treating x_2 as a constant. This will give you an integral over x_2 in which the exponent is a quadratic in x_2, so you can complete the square again to do this integral.]

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