Gaussian Integrals

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1 Motivation: Probability Distributions

To motivate the importance of Gaussian integrals, consider their most important application to probability theory used in thermodynamics. Thermodynamics considers macroscopic systems involving a large number (on the order of 10^{23}) of atomic or molecular particles: too many to individually describe the mechanics of each individual particle. Fortunately, thermodynamics is often interested in "average" quantities of an entire system, rather than the specifics of individual molecules. Because there are so many particles in the macroscopic systems studied by thermodynamics, the specifics values of quantities for individual molecules are often not relevant to the overall properties of a system, but rather their average values over many molecules. With this in mind, the specifics of individual particles can be ignored, and instead distribution for these quantities over the entire system is considered.

The distribution of a quantity can be described with a **probability density function**, or PDF. For a PDF $f(x)$, the $f(a)\mathrm{d}x$ is equal to the probability of measuring x between the values of a and $a + \mathrm{d}x$ in the distribution:

$$f(a)\mathrm{d}x = \text{probability of finding } x \text{ between } a \text{ and } a + \mathrm{d}x \tag{1.1}$$

The total probability of finding x within an interval $a < x < b$ is just the sum of $f(x)\mathrm{d}x$ for each x within that interval. This summation is just the integral from a to b of $f(x)\mathrm{d}x$:

$$\int_a^b f(x)\mathrm{d}x = \text{probability of finding } x \text{ between } a \text{ and } b \tag{1.2}$$

Some of the most common PDFs found in thermodynamics and modern physics are the **Gaussian function**

$$f(x) = Ae^{-\alpha x^2} \tag{1.3}$$

and a related set of functions containing the Gaussian function multiplied by some polynomial

$$f(x) = Ax^n e^{-\alpha x^2}, \tag{1.4}$$

where A and a are parameters for the Gaussian function. A **Gaussian integral** is the definite integral of the Gaussian function from $-\infty$ to ∞:

$$I = \int_{-\infty}^{\infty} Ae^{-\alpha x^2}\mathrm{d}x \tag{1.5}$$

When finding probabilities with a Gaussian PDF, the need to compute Gaussian integrals invariably comes up as a result of Equation (1.2). This handout examines methods for computing Gaussian integrals and presents several practice problems relevant to physics Olympiads.

2 Gaussian Integrals

To start, consider the simple case of a Gaussian integral I with $A = \alpha = 1$ in Equation (1.5):

$$I = \int_{-\infty}^{\infty} e^{-x^2}\mathrm{d}x \tag{2.1}$$

Unfortunately, the general antiderivative of $e^{-x^2}\mathrm{d}x$ can not be expressed in terms of elementary functions. However, the specific integral in Equation (2.1) can still be evaluated with a trick using polar coordinates.

Consider two Gaussian functions of two independent variables x and y. From basic probability theory, the probability of finding x within the range a_x to $a_x + \mathrm{d}x$ *and* y within the range a_y to $a_y + \mathrm{d}y$ is just the product of the individual probabilities for x and y

$$\left(e^{-x^2}\mathrm{d}x\right)\left(e^{-y^2}\mathrm{d}y\right) = \text{probability of finding } a_x < x < a_x + \mathrm{d}x \text{ and } a_y < x < a_y + \mathrm{d}y \tag{2.2}$$

This probability, which can be rewritten $\exp(-(x^2+y^2)) \times \mathrm{d}x \times \mathrm{d}y$, has the intuitive interpretation as the volume of a rectangular prism placed on the xy-plane. The total probability of finding any value of x and y is just the sum of these volumes for the entire xy-plane, which corresponds with the total volume V of the surface $z = \exp(-(x^2+y^2))$ over the entire xy-plane, shown in Figure **??**

However, because x and y are independent variables, basic probability theory states that the total probability of finding x and y anywhere on the xy-plane equal to the volume V is just equal the product of the probabilities of finding x between $-\infty$ and ∞ and y between the same interval, so

$$\left(\int_{-\infty}^{\infty} e^{-x^2}\mathrm{d}x\right)\left(\int_{-\infty}^{\infty} e^{-y^2}\mathrm{d}y\right) = V \tag{2.3}$$

However, the left-hand side of Equation (2.3) is just the product of two simple Gaussian integrals I! Then,

$$I^2 = V. \tag{2.4}$$

With Equation 2.4, the Gaussian integral can be solved by finding the volume under the surface $z = \exp(-(x^2+y^2))$ above the xy-plane. Fortunately, this volume is rotationally symmetric about the z-axis. This means the shell method of integration, shown schematically in Figure **??**, can be used. Splitting the volume into shells centered on the z-axis with radius r, the height z of each shell is:

$$z = e^{-\left(x^2+y^2\right)} = e^{-r^2}, \tag{2.5}$$

where the Pythagorean is used to make the substitution $r^2 = x^2 + y^2$. The thickness of each shell is $\mathrm{d}r$, and the circumference is $2\pi r$. Then, the shell volume $\mathrm{d}V$ is the product of the height, thickness, and circumference, or

$$\mathrm{d}V = 2\pi r e^{-r^2}\mathrm{d}r. \tag{2.6}$$

The total volume under the surface is then

$$V = \int_0^{\infty} 2\pi r e^{-r^2}\mathrm{d}r, \tag{2.7}$$

where the limits of integration from 0 to ∞ correspond to shells with radii from 0 to ∞ spanning the entire xy-plane. Because polar coordinates are used, there is an additional r factor in the integral, which allows it to be solved with u-substitution! Making the substitution $u = r^2$ gives

$$\begin{aligned}
V &= \int_0^{\infty} \frac{2\pi r}{2r} e^{-u}\mathrm{d}u \\
&= \int_0^{\infty} \pi e^{-u}\mathrm{d}u \\
&= -\pi e^{-u}\Big|_0^{\infty} \\
&= \pi
\end{aligned}$$

Then, substituting V into Equation (2.4) solves the Gaussian integral

$$\boxed{I = \sqrt{\pi}} \tag{2.8}$$

Example 1: Show that the general Gaussian integral is

$$I = \int_{-\infty}^{\infty} Ae^{-ax^2}\mathrm{d}x = A\sqrt{\frac{\pi}{a}}. \tag{2.9}$$

Solution 1: Again applying the polar substitution trick, the integral I boils down to finding a volume under the surface

$$I^2 = A^2\int_0^{\infty} 2\pi re^{-ar^2}\mathrm{d}r, \tag{2.10}$$

where the two factors of the constant A have been pulled out of the integral. Since there is an additional scaling factor a in the exponential, the u-substitution $u = ar^2$ is required. Then,

$$\begin{aligned} I^2 &= A^2\int_0^{\infty} \frac{2\pi r}{2ar}e^{-u}\mathrm{d}u \\ &= A^2\int_0^{\infty} \frac{\pi}{a}e^{-u}\mathrm{d}u \\ &= A^2\left(-\frac{\pi}{a}e^{-u}\Big|_0^{\infty}\right) \\ &= A^2\left(\frac{\pi}{a}\right), \end{aligned}$$

which means $\boxed{I = A\sqrt{\pi/a}}$.

Example 2: In thermodynamics, the Maxwell–Boltzmann velocity distribution describes the distribution of the velocities of molecules in an ideal gas. The PDF for the x-component of velocity v_x is given by:

$$f(v_x) = Ae^{-mv_x^2/2kT}, \tag{2.11}$$

where A is some scaling constant and the values of m, k, T are given for an ideal gas. The probability of finding any value of v_x from $-\infty$ to ∞ is just 1, since a molecule must have an x-component of velocity in that range. Therefore,

$$1 = \int_{-\infty}^{\infty} f(v_x)\mathrm{d}v_x. \tag{2.12}$$

Using Equation (2.12), find the expression for the scaling constant A.

Solution 2: $f(v_x)$ is a Gaussian function with $a = -m/2kT$. Applying the polar coordinate trick again (or just directly using the result from Example 2) gives

$$1 = A\sqrt{\frac{\pi}{m/2kT}}, \tag{2.13}$$

or

$$\boxed{A = \sqrt{\frac{m}{2\pi kT}}}. \tag{2.14}$$

3 Motivation: Expectation Values

Suppose you know the PDF $f(x)$ for some quantity x. One thing you might be interested in is the *average* or expectation value for x, denoted with the bracket notation $\langle x \rangle$, in some interval (a, b) of the distribution. For a non-uniform $f(x)$, some values of x will appear more often in the distribution than others, so the average would be a weighted sum of x multiplied by the probability of finding x at that value

$$\langle x \rangle = \sum_{x_i} x_i \cdot f(x_i) \mathrm{d}x, \tag{3.1}$$

where the summation is over all points $x_i \in (a, b)$. For a continuous distribution of x, Equation (3.1) can be rewritten with an integral

$$\langle x \rangle = \int_a^b x f(x) \mathrm{d}x. \tag{3.2}$$

Therefore, to find the expectation value for x or *any polynomial* for x in a Gaussian distribution in the interval $(-\infty, \infty)$, integrals of the form

$$\langle x^n \rangle = A \int_{-\infty}^{\infty} x^n e^{-ax^2} \mathrm{d}x \tag{3.3}$$

must be evaluated. Note that the expectation value of any polynomial of x in a Gaussian distribution is just a sum of separate x^n Gaussian integrals, since the integration operation is linear.

4 Related Gaussian Integrals

Consider the simple case were $n = 1$ and $A = a = 1$. The related Gaussian integral denoted I_1 is:

$$I_1 = \int_0^{\infty} x e^{-x^2} \mathrm{d}x \tag{4.1}$$

Note that the lower limit of integration has been set to 0 and the upper limit is the usual ∞. Since $x \exp(x^2)$ is an odd function, the integral from $(-\infty, \infty)$ is trivially zero and not particularly interesting.

Example 3: Show that $I_1 = 1/2$ in Equation (4.1).

Solution 3: I_1 can be easily evaluated using u-substitution.

$$\begin{aligned} I_1 &= \int_0^\infty x e^{-x^2} \mathrm{d}x \\ &= \int_0^\infty e^{-x^2} \frac{1}{2} \mathrm{d}x^2 \\ &= -\frac{1}{2} e^{-x^2} \Big|_0^\infty \\ &= \frac{1}{2} \end{aligned}$$

So $I_1 = 1/2$ as desired. Note that usual u-substitution has been written as

$$x \mathrm{d}x = \frac{1}{2} \mathrm{d}x^2. \tag{4.2}$$

This notation is just chosen for convenience and holds the same meaning as a $u = x^2$ substitution.

Now consider the integral I_2

$$I_2 = \int_{-\infty}^\infty x^2 e^{-x^2} \mathrm{d}x. \tag{4.3}$$

Unfortunately, direct u-substitution with $u = x^2$ will not work for Equation (4.3). Attempting u-substitution with x^2 as in Solution **??** gives

$$I_2 = \int_{-\infty}^\infty x e^{-x^2} \frac{1}{2} \mathrm{d}x^2. \tag{4.4}$$

The problem is that the integrand is $x \exp -x^2$, which contains an extra x factor. Fortunately, the standard way to evaluate this integral is to separate the product of x and e^{-x^2} using integration by parts to get

$$I_2 = -\frac{x e^{-x^2}}{2} \Bigg|_{-\infty}^\infty + \int_{-\infty}^\infty \frac{e^{-x^2}}{2} \mathrm{d}x. \tag{4.5}$$

The second term in Equation (4.5) is half of the simple Gaussian integral, giving $(\sqrt{\pi/a})/2$. Using L'Hôpital's rule, it can be shown that the first term is zero. Therefore,

$$I_2 = \frac{\sqrt{\pi}}{2}. \tag{4.6}$$

The process of performing u-substitution with integration parts can be repeated to find the expectation values of successively higher powers of x^n in a Gaussian distribution.

Example 4: Evaluate the integral

$$I_4 = \int_{-\infty}^\infty x^4 e^{-x^2} \mathrm{d}x. \tag{4.7}$$

Then, evaluate the general integral I_{2n} such that $n \in \mathbb{Z}$ is an integer

$$I_{2n} = \int_{-\infty}^{\infty} x^n e^{-x^2} \mathrm{d}x. \tag{4.8}$$

Solution 4: To evaluate I_4, first perform an x^2 substitution to give

$$I_4 = \int_{-\infty}^{\infty} x^3 e^{-x^2} \frac{1}{2} \mathrm{d}x^2 \tag{4.9}$$

Then, integration-by-parts gives

$$I_4 = -\frac{x^3 e^{-x^2}}{2}\bigg|_{-\infty}^{\infty} + \int_{-\infty}^{\infty} \frac{3x^2 e^{-x^2}}{2} \mathrm{d}x \tag{4.10}$$

Using L'Hôpital's rule, the first boundary term goes to zero. The second term is just $3/2 \cdot I_2$, so

$$\boxed{I_4 = \frac{3\sqrt{\pi}}{4}} \tag{4.11}$$

This procedure can be generalized to the integral I_{2n} with an even power of x in the Gaussian integral. All of the boundary terms from integration by parts will be in the form of some power of x multiplied with $\exp(-x^2)$ evaluated at $-\infty$ to ∞, which will go to zero by L'Hôpital's rule:

$$\text{boundary term} \propto x^m e^{-x^2}\bigg|_{-\infty}^{\infty} = 0. \tag{4.12}$$

Every time the substitution and integration by parts process is performed, the power of x^{2m} in the integral decreases by two, always remaining even until it reaches x^0 and the integral is reduced to a simple Gaussian integral. The integral term from integration by parts will acquire a factor of $1/2$ every time substitution is performed for each even power of x^{2m}, contributing a factor of

$$\text{substitution factor} = \frac{1}{2^n}. \tag{4.13}$$

For example, I_4 has $n = 2$, so Equation (4.13) accounts for the factor of $1/4$ found in expression for I_4 in Equation (4.11).

On the other hand, an odd factor $2m - 1$ that is one below the power x^{2m} will be multiplied every time integration by parts is performed, up until x^2. For example, the factor of 3 in the expression for I_4 in Equation (4.11) is account for by the product of 3×1, since 3 and 1 are both one less than the x^4 and x^2. This product of odd powers can be expressed for any general I_{2n} as

$$\text{integration by parts factor} = \frac{(2n-1)!}{2^{n-1}(n-1)!}. \tag{4.14}$$

The $(2n - 1)!$ in the numerator accounts for all of the odd factors that are one less than $2n$, but also includes the even factors. There are $n - 1$ of these even factors starting from 2, so they can be removed by dividing by $(n - 1)!$ scaled by factors of two with 2^{n-1}.

Combining the factors Equation (4.13) and Equation (4.14) with the value of the standard Gaussian integral at the end of the substitution and integration by parts process gives

$$I_{2n} = \frac{(2n-1)!}{2^{2n-1}(n-1)!}\sqrt{\pi}. \tag{4.15}$$