QM Handout – Gaussian Integration

Gaussian integration is simply integration of the exponential of a quadratic. We cannot write a simple expression for an indefinite integral of this form but we can find the exact answer when we integrate from $-\infty$ to ∞. The basic integral we need is

$$G \equiv \int_{-\infty}^{\infty} dx e^{-x^2}$$

The trick to calculate this is to square this using integration variables x and y for the two integrals and then evaluate the double integral using polar coordinates. N.B. from now on we will simply drop the range of integration for integrals from $-\infty$ to ∞. So

$$G^2 = \int dx e^{-x^2} \int dy e^{-y^2} = \int dx \int dy e^{-(x^2+y^2)}$$

$$= \int_0^{2\pi} d\theta \int_0^{\infty} dr r e^{-r^2} = 2\pi \int_0^{\infty} \frac{1}{2} d(r^2) e^{-r^2} = \pi$$

This gives the important result

$$\int dx e^{-x^2} = \sqrt{\pi}$$

For a real constant $a > 0$ a change of variables gives

$$G(a) \equiv \int dx e^{-ax^2} = \frac{1}{\sqrt{a}} \int d(\sqrt{a}x) e^{-(\sqrt{a}x)^2} = \sqrt{\frac{\pi}{a}}$$

For a general quadratic exponent we simply complete the square and then integrate using a similar change of variables

$$\int dx e^{-ax^2+bx+c} = \int dx e^{-a(x-\frac{b}{2a})^2} e^{\frac{b^2}{4a}+c} = \sqrt{\frac{\pi}{a}} e^{\frac{b^2}{4a}+c}$$

These results extend to the case of complex numbers a, b and c provided the real part of a is positive. We can also consider the case where a is purely imaginary (but non-zero) which can be justified by first multiplying the integrand by $e^{-\epsilon x^2}$ for positive real ϵ, and then taking the limit $\epsilon \to 0$ after integrating.

Now we can also calculate integrals involving a polynomial times the exponential of a quadratic. By completing the square for the quadratic we can reduce such an integral to a sum of integrals of the form

$$\int dx x^N e^{-ax^2}$$

where N is a non-negative integer and, restricting to real coefficients, the constant a must be positive for the integral to be well-defined. We can easily calculate this integral using integration by parts, integrating xe^{-ax^2} and differentiating x^{N-1}. This relates the integral to another of the same type but with N replaced by $N-2$, giving a recursion relation. Using this method we get the following results for non-negative integers n:

$$\int_{-\infty}^{\infty} dx x^{2n} e^{-ax^2} = \frac{(2n-1)(2n-3)\cdots 3\cdot 1}{(2a)^n}\sqrt{\frac{\pi}{a}} \tag{1}$$

$$\int_{-\infty}^{\infty} dx x^{2n+1} e^{-ax^2} = 0 \tag{2}$$

$$\int_{0}^{\infty} dx x^{2n} e^{-ax^2} = \frac{1}{2}\frac{(2n-1)(2n-3)\cdots 3\cdot 1}{(2a)^n}\sqrt{\frac{\pi}{a}} \tag{3}$$

$$\int_{0}^{\infty} dx x^{2n+1} e^{-ax^2} = \frac{n!}{2a^{n+1}} \tag{4}$$

Note that by symmetry, results (1) and (3) are related by a factor of 2 since the integrand is an even function, while result (2) follows from the integrand being an odd function.

It is also possible to derive these results by considering a to be a variable and differentiating with respect to a. For example starting with

$$G(a) \equiv \int dx e^{-ax^2} = \sqrt{\frac{\pi}{a}}$$

and differentiating with respect to a we get

$$G'(a) = \int dx(-x^2)e^{-ax^2} = -\frac{1}{2}\frac{\sqrt{\pi}}{a^{3/2}}$$

which gives

$$\int dx x^2 e^{-ax^2} = \frac{\sqrt{\pi}}{2a^{3/2}}$$

in agreement with result (1) for $n=1$.

As an aside, you will have noticed the $n!$ appearing in result (4) and the somewhat similar product in result (3), after dividing the numerator by 2^n

$$(n-\frac{1}{2})(n-\frac{3}{2})\cdots\frac{3}{2}\cdot\frac{1}{2}$$

Indeed we can define a complex function, known as the gamma function, which can be viewed as an extension of the factorial function, by

$$\Gamma(z) = 2\int_0^{\infty} dx x^{2z-1}e^{-x^2}$$

for $\Re(z) > 0$ which satisfies the recurrence relation

$$z\Gamma(z) = \Gamma(z+1)$$

This recurrence relation allows us to extend the definition to all $z \in \mathbf{C}$ and from result (4) we see that for any positive integer n, $\Gamma(n) = (n-1)!$.