8.4: Double and Triple Integrals

We can extend the idea of a definite integral to more dimensions. If $f(x,y)$ is continuous over the rectangle $R=[a,b]\times[c,d]$ then,

$$\iint_R f(x,y)dA=\int_a^b\int_c^d f(x,y)\,dy\,dx=\int_c^d\int_a^b f(x,y)\,dx\,dy \tag{8.4.1}$$

If $f(x,y)\geq 0$, then the double integral represents the volume V of the solid that lies above the rectangle R and below the surface $z=f(x,y)$ (Figure 8.4.1).

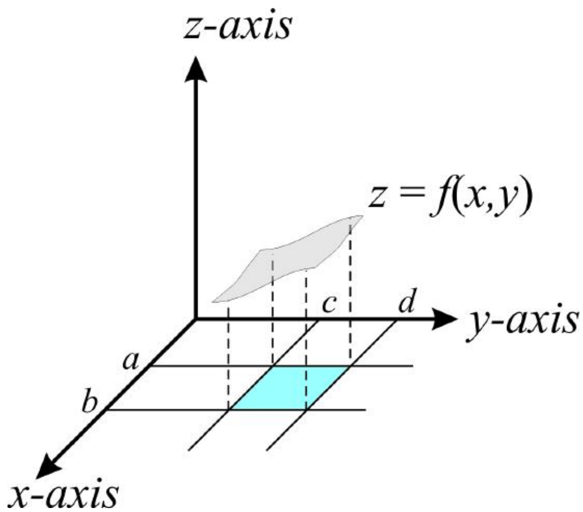

Figure 8.4.1: Geometric interpretation of a double integral (CC BY-NC-SA; Marcia Levitus)

We can compute the double integral of Equation 8.4.1 as:

$$\iint_R f(x,y)dA=\int_a^b\left[\int_c^d f(x,y)\,dy\right]dx$$

meaning that we will first compute

$$\int_c^d f(x,y)\,dy$$

holding x constant and integrating with respect to y. The result will be a function containing only x, which we will integrate between a and b with respect to x.

For example, let's solve $\int_0^3\int_1^2 x^2y\;dy\;dx$. We'll start by solving $\int_1^2 x^2y\;dy$ holding x constant:

$$\int_1^2 x^2y\;dy=x^2\int_1^2 y\;dy=\frac{3}{2}x^2$$

Now we integrate this function from 0 to 3 with respect to x:

$$\int_0^3\int_1^2 x^2y\;dy\;dx=\int_0^3\frac{3}{2}x^2\;dx=\frac{27}{2}$$

You can of course integrate from 0 to 3 first with respect to x holding y constant, and then integrate the result with respect to y from 1 to 2. Try it this way and verify you get the same result.

Triple integrals work in the same way. If $f(x,y,z)$ is continuous on the rectangular box $B=[a,b]\times[c,d]\times[r,s]$, then

$$\iiint_B f(x,y,z)dV=\int_r^s\int_c^d\int_a^b f(x,y)\,dx\,dy\,dz \tag{8.4.2}$$

This iterated integral means that we integrate first with respect to x (keeping y and z fixed), then we integrate with respect to y (keeping z fixed), and finally we integrate with respect to z. There are five other possible orders in which we can integrate, all of which give the same value.

> Do you need a refresher on double and triple integrals? Check the videos below before moving on to the physical chemistry examples.
>
> - Example 1: http://www.youtube.com/watch?v=RqD89-afGS0
> - Example 2: http://www.youtube.com/watch?v=CPR0ZD0IYVE (check the example that starts around 3:45 min. and ends at 5:07 min)

Triple integrals are used very often in physical chemistry to normalize probability density functions. For example, in quantum mechanics, the absolute square of the wave function, $|\psi(x,y,z)|^2$, is interpreted as a *probability density*, the probability that the particle is inside the volume $dx.dy.dz$. Since the probability of finding the particle somewhere in space is 1, we require that:

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}|\psi(x,y,z)|^2\,dx\,dy\,dz=1 \tag{8.4.3}$$

We already mentioned wave functions in Section 2.3, where we showed that

$$|\psi(x,y,z)|^2=\psi^*(x,y,z)\psi(x,y,z)$$

The normalization condition, therefore, can also be written as

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\psi^*\psi\,dx\,dy\,dz=1 \tag{8.4.4}$$

Example 8.4.1

In quantum mechanics, the lowest energy state of a particle confined in a three-dimensional box is represented by

$$\psi(x,y,z)=A\sin\frac{\pi x}{a}\sin\frac{\pi y}{b}\sin\frac{\pi z}{c}\ if\begin{cases}0<x<a\\0<y<b\\0<z<c\end{cases}$$

and

$$\psi(x,y,z)=0 \text{ otherwise (outside the box).}$$

Here, A is a normalization constant, and a,b and c are the lengths of the sides of the box. Since the probability of finding the particle somewhere in space is 1, we require that

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}|\psi(x,y,z)|^2\,dx\,dy\,dz=1$$

Find the normalization constant A in terms of a,b,c and other constants.

Solution

Because $\psi(x,y,z)=0$ outside the box,

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}|\psi(x,y,z)|^2\,dx\,dy\,dz=\int_0^c\int_0^b\int_0^a|\psi(x,y,z)|^2\,dx\,dy\,dz=|\psi(x,y,z)|^2=\psi^*(x,y,z)\psi(x,y,z)$$

However, because in this case the function is real,

$$|\psi(x,y,z)|^2=(\psi(x,y,z))^2$$

$$\int_0^c\int_0^b\int_0^a|\psi(x,y,z)|^2\,dx\,dy\,dz=\int_0^c\int_0^b\int_0^a A^2\sin^2\left(\frac{\pi x}{a}\right)\sin^2\left(\frac{\pi y}{b}\right)\sin^2\left(\frac{\pi z}{c}\right)\,dx\,dy\,dz=1$$

$$\int_0^c \int_0^b \int_0^a A^2 \sin^2\left(\frac{\pi x}{a}\right) \sin^2\left(\frac{\pi y}{b}\right) \sin^2\left(\frac{\pi z}{c}\right)\, dx\; dy\; dz = A^2 \int_0^a \sin^2\left(\frac{\pi x}{a}\right) dx \int_0^b \sin^2\left(\frac{\pi y}{b}\right) dy \int_0^c \sin^2\left(\frac{\pi z}{c}\right) dz$$

Using the formula sheet, we get

$$\int_0^a \sin^2\left(\frac{\pi x}{a}\right) dx = a/2$$

And therefore,

$$A^2 \int_0^a \sin^2\left(\frac{\pi x}{a}\right) dx \int_0^b \sin^2\left(\frac{\pi y}{b}\right) dy \int_0^c \sin^2\left(\frac{\pi z}{c}\right) dz = A^2 \frac{a}{2}\frac{b}{2}\frac{c}{2} = \frac{A^2 abc}{8} = 1$$

Solving for A:

$$A = \left(\frac{8}{abc}\right)^{1/2}$$