CHEM2024 - Week 22 Lecture 2 - Multiple integrals in Cartesian coordinates

Sections 9.8-9.10 of Steiner, "The Chemistry Maths Book", 2nd edition.

Pages 376-382 of Monk and Munro, "Maths for Chemistry", 2nd edition.

Just as partial differentiation was carried out by assuming all other variables to be constants, integration with respect to just one of many variables may be carried out by treating all other variables as constants, assuming that the function remains integrable for all values that those other variables can take, *e.g.*:

$$\int_0^1 x\cos(y)\,dx = \cos(y)\int_0^1 x\,dx = \left.\frac{x^2}{2}\right|_{x=0}^{x=1}\cos(y) = \frac{1}{2}\cos(y)$$

Multiple indefinite integrals accumulate constants in a way that depends on the order of integration:

$$\iiint x\,dx\,dy\,dz = \iint\left(\frac{x^2}{2}+C_1\right)dy\,dz = \int\left(\frac{x^2 y}{2}+C_1 y + C_2\right)dz = \frac{x^2 yz}{2}+C_1 yz + C_2 z + C_3$$

By convention, the inner integral is evaluated first. To make notation less awkward, the standard way of writing multiple integrals is to list the integration operations one after the other – the integral that is nearest to the function should be evaluated first:

$$\int_1^2\int_0^1 xy\,dx\,dy = \int_1^2 dy\int_0^1 xy\,dx$$

This is an example of operator notation: the formula on the right asks the user to take xy, integrate it from 0 to 1 with respect to x and then integrate the result from 1 to 2 with respect to y.

1. Multiple integrals with explicit limits

When limits are specified explicitly, multiple integrals can be taken one after the other. Example:

$$\int_1^2 dy\int_0^1 (xy)\,dx = \int_1^2 y\left(\left.\frac{x^2}{2}\right|_{x=0}^{x=1}\right)dy = \frac{1}{2}\int_1^2 y\,dy = \left.\frac{1}{2}\frac{y^2}{2}\right|_{y=1}^{y=2} = \frac{3}{4}$$

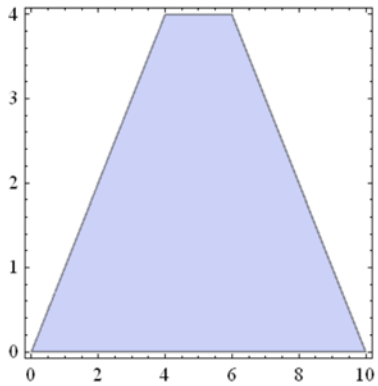
Integration limits need not be constants – they can depend on the variable that is integrated over at a later point. The Newton-Leibnitz formula should be used in the same way. Example:

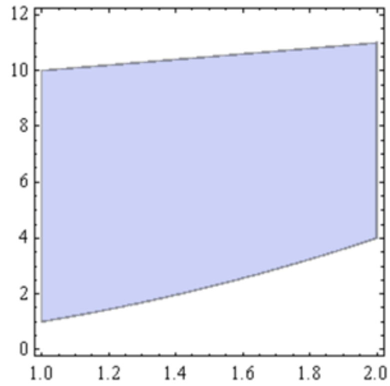
$$\int_{-3}^{3} dy \int_{y^2-4}^{5}(x+2y)\,dx = \int_{-3}^{3} dy\left.\left(\frac{x^2}{2}+2xy\right)\right|_{x=y^2-4}^{x=5} = \int_{-3}^{3} dy\left(\frac{25}{2}+10y-\frac{(y^2-4)^2}{2}-2(y^2-4)y\right) =$$

$$= \int_{-3}^{3} dy\left(\frac{9}{2}+18y+4y^2-2y^3-\frac{y^4}{2}\right) = \ldots = \frac{252}{5}$$

The presence of variable limits indicates that the region over which the integration is performed is not rectangular, for example:

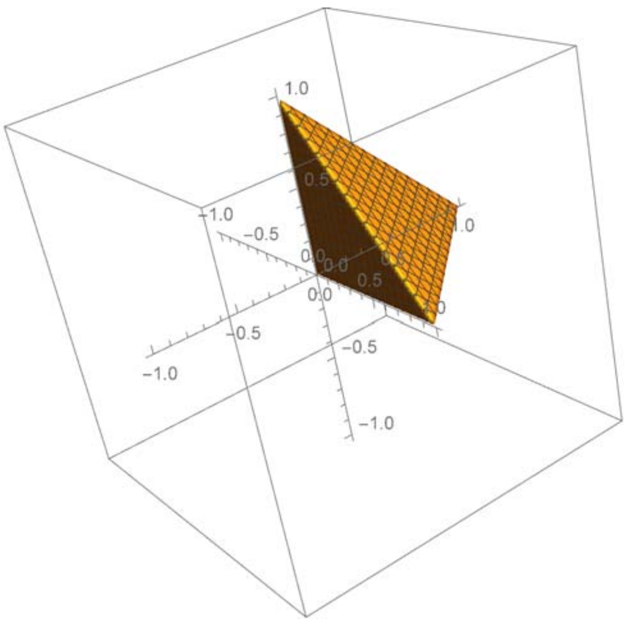
$$\int_0^4 dy \int_y^{10-y} f(x,y)\,dx \qquad\qquad \int_1^2 dx \int_{x^2}^{x+9} f(x,y)\,dy$$





2. Multiple integrals over implicitly defined domains

When the integration region is specified implicitly, the variable integration limits should be established by analysing the corresponding geometric area or volume.

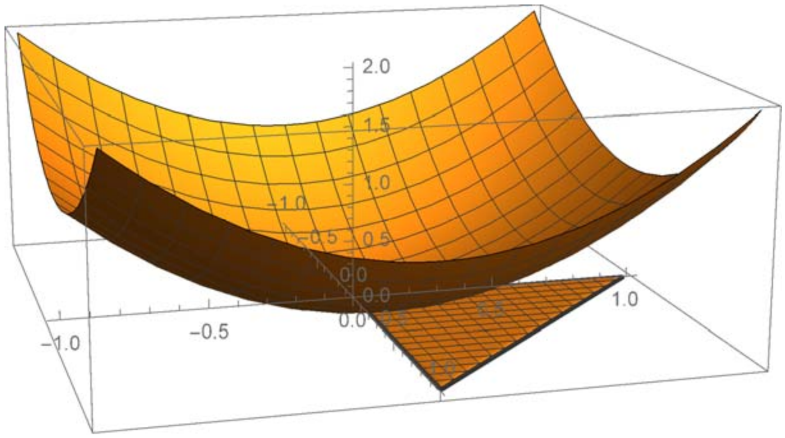


For example, a triple integral of a function $f(x,y,z)$ over the volume bounded by the three Cartesian planes and the triangle defined by $[1,0,0]$, $[0,1,0]$ and $[0,0,1]$ – shown in Figure 2 above – would yield the following integration limits:

$$\int_0^1 dx \int_0^{1-x} dy \int_0^{1-x-y} f(x,y,z)\,dz$$

because all three integration variables are positive, x may be chosen to vary between 0 and 1, then y must vary between 0 and $1-x$, and then z must vary between 0 and $1-x-y$. Because the upper limit with respect to z depends on other variables, the z integral must be taken first, then y integral (whose upper limit depends on x, and then finally the x integral.

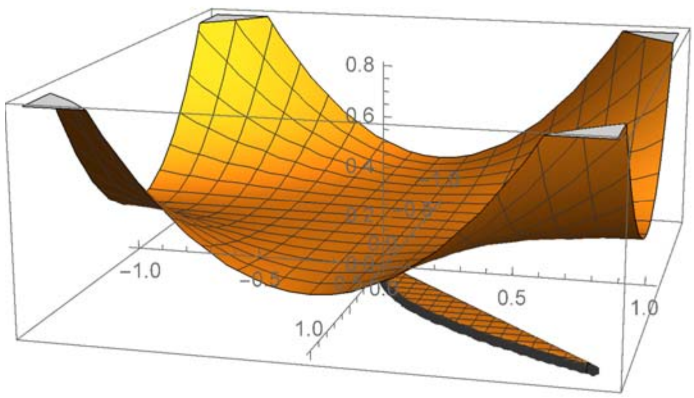
Example 1: integrate the function $f(x,y) = x^2 + y^2$ over the area bounded by the two Cartesian axes and a triangle defined by $[0,0]$, $[1,0]$ and $[0,1]$.



Solution: the analysis of the integration region produces the following double integral

$$\int_0^1 dy \int_0^{1-y} \left(x^2 + y^2\right) dx = \int_0^1 dy \left(\frac{x^3}{3} + xy^2\right)\Bigg|_{x=0}^{x=1-y} = \int_0^1 \left(\frac{(1-y)^3}{3} + (1-y)\,y^2\right) dy = \ldots = \frac{1}{6}$$

Example 2: integrate the function $f(x,y) = y^2 x^2$ over the area bounded by $y = x$ and $y = x^2$.



Solution: the analysis of the integration region produces the following double integral

$$\int_0^1 dx \int_{x^2}^{x} y^2 x^2 dy = \int_0^1 dx \left(\frac{y^3}{3} x^2\right)\Bigg|_{x^2}^{x} = \frac{1}{3}\int_0^1 \left(x^3 - x^6\right) x^2 dx = \ldots = \frac{1}{54}$$

If the functions are chosen to be $f(x,y) = 1$ or $f(x,y,z) = 1$, the corresponding integrals return the area and the volume, respectively, of the integration domain.