CHEM1034 - Week 24 Lecture - Multivariate functions: integration

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.

Line integrals

A problem that often presents itself in chemical thermodynamics and physics in general is the calculation of an integral over an arbitrary smooth curve, for instance:

$$\int_C \left[f(x,y)\,dx + g(x,y)\,dy \right] \tag{1}$$

A good example of such an integral is the change in internal energy of a chemical system going through a thermodynamic process specified by a curve C in the $\{P,V,T\}$ parameter space:

$$dU = TdS - PdV \quad \Rightarrow \quad \Delta U = \int_C [TdS - PdV] \tag{2}$$

Another example is the work W done by a particle moving along a curve C in three dimensions against a force $\vec{f} = \begin{bmatrix} f_X & f_Y & f_Z \end{bmatrix}$, which is given by the following integral:

$$W = \int_C \left[f_X(x,y,z)\,dx + f_Y(x,y,z)\,dy + f_Z(x,y,z)\,dz \right] \tag{3}$$

The integration curve C would normally be parameterised by some common variable, for example time:

$$x = x(t), \qquad y = y(t), \qquad a \le t \le b \tag{4}$$

In that case, $dx = x'(t)dt$ and $dy = y'(t)dt$ – the line integral in Equation (1) gets reduced to an ordinary integral with respect to time:

$$\begin{aligned} \int_C \left[f(x,y)\,dx + g(x,y)\,dy \right] &= \int_C \left[f(x,y)\,x'(t)\,dt + g(x,y)\,y'(t)\,dt \right] = \\ &= \int_a^b \left[f\big(x(t),y(t)\big)\,x'(t) + g\big(x(t),y(t)\big)\,y'(t) \right] dt \end{aligned} \tag{5}$$

<u>Example</u>: compute the following integral

$$\int_C [yzdx + xzdy + xydz]$$

over the curve specified by $\begin{bmatrix} x(t) & y(t) & z(t) \end{bmatrix} = \begin{bmatrix} t & t^2 & t^3 \end{bmatrix}$ for $0 \le t \le 1$.

<u>Solution</u>: the differentials of the three Cartesian coordinates are

$$dx = dt, \qquad dy = 2tdt, \qquad dz = 3t^2dt$$

Performing the corresponding substitution under the integral yields:

$$\int_C [yzdx + xzdy + xydz] = \int_0^1 \left[yzdt + 2xztdt + 3xyt^2dt \right] = \int_0^1 6t^5dt = 1$$

Multiple integrals in Cartesian coordinates

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.*:

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

further integrals with respect to other variables can then be taken if necessary. Note that multiple indefinite integrals would accumulate arbitrary 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:

$$\int_1^2\left[\int_0^1 (xy)\,dx\right]dy = \int_1^2 dy\int_0^1 (xy)\,dx$$

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.

In simple cases multiple integrals can be taken directly, by evaluating each integral in sequence. Example:

$$\int_1^2 dy\int_0^1 dx[xy] = \int_1^2\left[\int_0^1 (xy)\,dx\right]dy = \int_1^2 y\left[\int_0^1 x\,dx\right]dy = \int_1^2 y\left[\frac{x^2}{2}\Bigg|_0^1\right]dy = \frac{1}{2}\int_1^2 y\,dy = \frac{1}{2}\left[\frac{y^2}{2}\Bigg|_1^2\right] = \frac{3}{4}$$

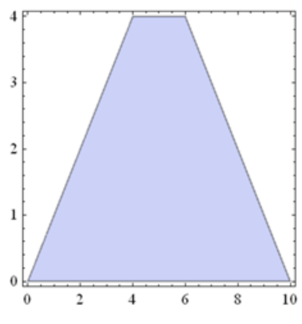
Integration limits need not be constants – they can depend on the variable that is integrated over at a later point. The Newton-Leibniz formula should be used in the same way. Example:

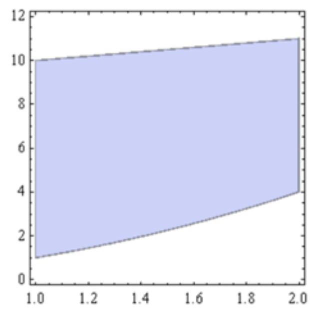
$$\int_{-3}^{3} dy\int_{y^2-4}^{5}(x+2y)\,dx = \int_{-3}^{3} dy\left(\frac{x^2}{2}+2xy\right)\Bigg|_{x=y^2-4}^{x=5} = \int_{-3}^{3} dy\left(\frac{25}{2}+10y-\frac{\left(y^2-4\right)^2}{2}-2\left(y^2-4\right)y\right) =$$

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

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

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





When the integration region is specified implicitly, the variable integration limits should be established by analysing the corresponding geometric area. 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 $[0,0,1]$ would yield the following integration limits:

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

Example: 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: 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

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

In particular, 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 for the integration domain.

Week 25 workshop exercises

Monk and Munro, 2nd edition: problems 26.2-26.6.

Steiner, 2nd edition: Section 9.12, problems 57-60, 64, 66-68.

Extra difficulty exercises for the brave

Steiner, 2nd edition: section 10.7, problems 14-17, 34.