CHEM2024 - Week 23 Lecture 2 - Integration in curvilinear coordinates

Chapter 16 of Monk and Munro, "Maths for Chemistry", 2nd edition.
Section 3.5 and Chapter 10 of Steiner, "The Chemistry Maths Book", 2nd edition.

Integrating in polar and spherical coordinates is not as simple as changing variables and updating integration limits: the volume element $dxdydz$ is the same everywhere, but the volume element $drd\theta d\varphi$ is different in different locations – this is illustrated in Figure 1. The same applies to the area element $dxdy$ and its polar equivalent $drd\varphi$.

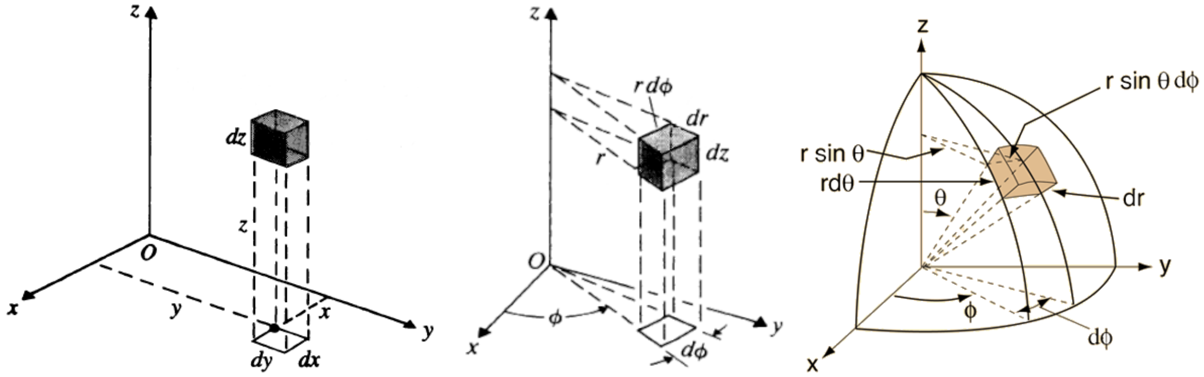


***Figure 1.** Volume elements in Cartesian (left), cylindrical (middle), and spherical (right) coordinates. The size of the volume is only location-independent in Cartesian coordinates.*

To take integrals in polar and spherical coordinates, we must therefore find a way to transform volume elements from one coordinate system into another.

1. Jacobian matrix

We need to determine how the expression for the volume of an infinitesimally small hypercube is transformed when we move from one coordinate system into another:

$$\begin{cases} x = x(u, v, ...) \\ y = y(u, v, ...) \\ ... \end{cases} \tag{1}$$

It may be shown (we do not have the time for the full derivation here) that

$$dxdy... = \det \begin{bmatrix} \partial x/\partial u & \partial x/\partial v & \cdots \\ \partial y/\partial u & \partial y/\partial v & \cdots \\ \vdots & \vdots & \ddots \end{bmatrix} dudv... \tag{2}$$

The matrix of partial derivatives is called *Jacobian matrix*. Its determinant is used for volume element transformation when moving integrals between different coordinate systems.

2. Polar and cylindrical integrals

Moving to polar or cylindrical coordinates is beneficial when a physical system or a mathematical expression have rotational symmetry around a single axis. From the definition of polar coordinates:

$$\begin{cases} x = r\cos\varphi \\ y = r\sin\varphi \end{cases} \tag{3}$$

we can obtain the Jacobian matrix determinant

$$\mathbf{J}(r,\varphi)=\begin{bmatrix}\dfrac{\partial x}{\partial r} & \dfrac{\partial x}{\partial \varphi}\\ \dfrac{\partial y}{\partial r} & \dfrac{\partial y}{\partial \varphi}\end{bmatrix}=\begin{bmatrix}\cos\varphi & -r\sin\varphi\\ \sin\varphi & r\cos\varphi\end{bmatrix},\qquad \det[\mathbf{J}]=r \tag{4}$$

Therefore, the relationship between the volume elements is

$$dxdy = rdrd\varphi \tag{5}$$

Example 1: integrate $f(x,y)=1/(1+x^2+y^2)$ over the disk of radius 1 with the centre at the origin.

Solution: an attempt to take this integral in Cartesian coordinates is unlikely to succeed

$$\iint_{\text{disk}}\frac{1}{1+x^2+y^2}dxdy=\int_{-1}^{1}dx\int_{-\sqrt{1-x^2}}^{+\sqrt{1-x^2}}\frac{dy}{1+x^2+y^2}=\ldots$$

However, the disk has rotational symmetry and x^2+y^2 has a particularly simple form in polar coordinates: $x^2+y^2=r^2(\cos^2\varphi+\sin^2\varphi)=r^2$. The integration limits also become simple in polar coordinates:

$$\iint_{\text{disk}}\frac{1}{1+x^2+y^2}dxdy=\int_0^1 dr\int_0^{2\pi}\frac{r}{1+r^2}d\varphi$$

where the extra r appeared in the outer integral because of the relationship between $dxdy$ and $drd\varphi$ given in Equation (5). The integral is now easy to take:

$$\int_0^1 dr\int_0^{2\pi}\frac{r}{1+r^2}d\varphi=2\pi\int_0^1\frac{rdr}{1+r^2}=\begin{Bmatrix}\text{subst:}\\ x=r^2\end{Bmatrix}=\pi\int_0^1\frac{dx}{1+x}=\pi\ln 2$$

Cylindrical coordinates have one Cartesian component that does not participate in the curvilinear transformation because it only contributes a unit element on the diagonal of the matrix:

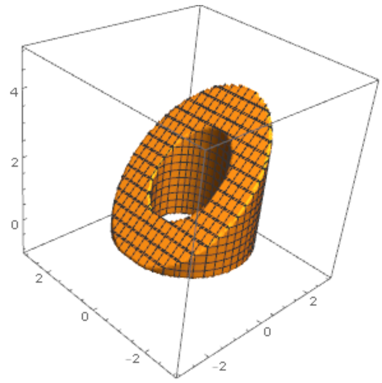
$$\mathbf{J}(r,\varphi,h)=\begin{bmatrix}\partial x/\partial r & \partial x/\partial\varphi & 0\\ \partial y/\partial r & \partial y/\partial\varphi & 0\\ 0 & 0 & 1\end{bmatrix}=\begin{bmatrix}\cos\varphi & -r\sin\varphi & 0\\ \sin\varphi & r\cos\varphi & 0\\ 0 & 0 & 1\end{bmatrix},\qquad \det[\mathbf{J}]=r \tag{6}$$

and therefore the relationship between the volume elements for cylindrical coordinates is:

$$dxdydz = rdrd\varphi dh \tag{7}$$

Example 2: integrate $f(x,y,z)=y$ over the volume that lies below the plane $z=x+2$, above the XY plane, and between the cylinders $x^2+y^2=1$ and $x^2+y^2=4$.

Solution: sketching the integration volume indicates that the problem has cylindrical symmetry



with the radius vector scanning the $1 \le r \le 2$ interval, the polar angle doing the complete sweep and the z coordinate going from zero to $x+2$. We can now take the integral:

$$\int_0^{2\pi} d\varphi \int_1^2 r dr \int_0^{r\cos\varphi+2} r\sin\varphi dh = [\ldots] = 0$$

3. Spherical integrals

Moving to spherical coordinates is recommended when integrals are taken in the context of spherical rotation symmetry (atoms, spins, *etc.*). From the definition of spherical coordinates:

$$\begin{cases} x = r\sin\theta\cos\varphi \\ y = r\sin\theta\sin\varphi \\ z = r\cos\theta \end{cases} \qquad (8)$$

we can obtain the Jacobian matrix and its determinant

$$\mathbf{J}(r,\theta,\varphi) = \begin{bmatrix} \frac{\partial x}{\partial r} & \frac{\partial x}{\partial \theta} & \frac{\partial x}{\partial \varphi} \\ \frac{\partial y}{\partial r} & \frac{\partial y}{\partial \theta} & \frac{\partial y}{\partial \varphi} \\ \frac{\partial z}{\partial r} & \frac{\partial z}{\partial \theta} & \frac{\partial z}{\partial \varphi} \end{bmatrix} = \begin{bmatrix} \sin\theta\cos\varphi & r\cos\theta\cos\varphi & -r\sin\theta\sin\varphi \\ \sin\theta\sin\varphi & r\cos\theta\sin\varphi & r\sin\theta\cos\varphi \\ \cos\theta & -r\sin\theta & 0 \end{bmatrix} \qquad (9)$$

$$\det[\mathbf{J}] = r^2\sin\theta$$

and therefore the relationship between the volume elements is

$$dxdydz = r^2\sin\theta dr d\theta d\varphi \qquad (10)$$

<u>Example 3</u>: integrate $f(x,y,z) = 4z$ over the upper half of the sphere defined by $x^2+y^2+z^2=1$.

<u>Solution</u>: we would not attempt to write this integral in its Cartesian form and move straight into spherical coordinates, not forgetting the Jacobian:

$$\int_0^{2\pi} d\varphi \int_0^{\pi/2} \sin\theta d\theta \int_0^1 (4r\cos\theta) r^2 dr = 2\pi \int_0^{\pi/2} \cos\theta\sin\theta d\theta \int_0^1 4r^3 dr =$$

$$= 2\pi \int_0^{\pi/2} \cos\theta\sin\theta d\theta \left[1^4 - 0^4\right] = 2\pi \int_0^{\pi/2} \cos\theta\sin\theta d\theta = \begin{Bmatrix} \text{subst:} \\ x = \sin\theta \end{Bmatrix} = 2\pi \int_0^1 x dx = \pi$$