CHEM1047 - Week 10 Lecture 1 - Integration, Part II

☐ *Chapters 23-25 of Monk and Munro, "Maths for Chemistry", 2nd edition.*

☐ *Chapter 6 of Steiner, "The Chemistry Maths Book", 2nd edition.*

1. Integration by substitution

Let $f(u)$ and $u=\varphi(x)$ be differentiable functions. Then, if $f(u)$ has an antiderivative $F(u)$, then $f(\varphi(x))\varphi'(x)$ has an antiderivative $F(\varphi(x))+C$ and thus

$$\int f(\varphi(x))\varphi'(x)\,dx = F(\varphi(x))+C \tag{1}$$

Proof: using the chain rule to differentiate the antiderivative back,

$$\frac{d}{dx}F(\varphi(x)) = \frac{d}{d\varphi}F(\varphi)\frac{d}{dx}\varphi(x) = f(\varphi)\varphi'(x) \tag{2}$$

we can demonstrate that Equation (1) is correct.

Example 1: consider the following integral

$$\int (3x+4)^5\,dx \tag{3}$$

Solution: the table of standard integrals contains no obvious rules that would allow us to integrate this expression. However, we can perform the following substitution:

$$y = 3x+4 \tag{4}$$

Computing the differential provides the connection between dx and dy:

$$dy = 3dx \quad\Rightarrow\quad dx = dy/3 \tag{5}$$

Performing the substitutions in Equation (3) results in the following integral

$$\frac{1}{3}\int y^5 dy \tag{6}$$

which can be taken directly:

$$\frac{1}{3}\int y^5 dy = \frac{1}{18}y^6 + C \tag{7}$$

Using Equation (4) to convert y back into $3x+4$ produces the final answer:

$$\int (3x+4)^5\,dx = \frac{1}{18}(3x+4)^6 + C \tag{8}$$

The correctness of this answer may be verified by differentiating the result:

$$\left[\frac{1}{18}(3x+4)^6 + C\right]' = [\ldots] = (3x+4)^5 \tag{9}$$

Example 2: consider the following integral

$$\int x\sqrt{1+x^2}\,dx \tag{10}$$

Solution: the problematic part here that prevents us from taking the integral is the expression under the square root. Let us try performing the following substitution:

$$y=1+x^2 \quad \Rightarrow \quad dy=2xdx \quad \Rightarrow \quad dx=\frac{dy}{2x} \tag{11}$$

Performing this substitution makes the variable x disappear from the integral

$$\int x\sqrt{1+x^2}dx=\int x\sqrt{y}\frac{dy}{2x}=\frac{1}{2}\int y^{1/2}dy \tag{12}$$

This integral is easy to take using the table above:

$$\frac{1}{2}\int y^{1/2}dy=\frac{1}{2}\frac{2}{3}y^{3/2}+C=\frac{1}{3}y^{3/2}+C \tag{13}$$

Back-substitution yields the final answer:

$$\int x\sqrt{1+x^2}dx=\frac{1}{3}\left(1+x^2\right)^{3/2}+C \tag{14}$$

Note that variable substitution does not always lead to a simplification because the presence of $\varphi'(x)$ term can introduce additional complications. If variable substitution fails, other integration methods should be tried. Note also that indefinite integrals must always be brought back to the original variables after the integration process is finished.

For definite integrals, the variable substitution formula is modified to account for the fact that integration limits change when the integration is performed over a function of the original variable:

$$\int_a^b f(x)dx=\int_{u(a)}^{u(b)}\left[f(u)\left(\frac{du}{dx}\right)^{-1}\right]du \tag{15}$$

Example 4: calculate the integral of $1/(4x+5)^4$ from $x=0$ to $x=1$.

Solution: the integral would simplify if we use $u=4x+5$ substitution

$$\int_0^1\frac{1}{(4x+5)^4}dx=\begin{bmatrix}u=4x+5 & du=4dx\\ u(0)=5 & u(1)=9\end{bmatrix}=\int_5^9\left[\frac{1}{u^4}\cdot\frac{1}{4}\right]du=\frac{1}{4}\int_5^9 u^{-4}du=$$

$$=\frac{1}{4}\frac{1}{-3}u^{-3}\Big|_5^9=-\frac{1}{12}\left(9^{-3}-5^{-3}\right)=\frac{151}{273375}$$

2. Integration by parts

If $u(x)$ and $v(x)$ are differentiable in some interval and their integrals exist, then:

$$\int_a^b u(x)v'(x)dx=\left[u(x)v(x)\right]\Big|_a^b-\int_a^b u'(x)v(x)dx \tag{16}$$

A shorthand form of this rule that is easy to memorise is:

$$\int udv=uv-\int vdu \tag{17}$$

<u>Proof</u>: calculating the differential of the product $u(x)v(x)$ yields

$$d\left[u(x)v(x)\right]=u'(x)v(x)dx+u(x)v'(x)dx \tag{18}$$

After integrating both sides from a to b and rearranging the terms, we get:

$$\int_a^b u(x)v'(x)dx = \int_a^b d\left[u(x)v(x)\right] - \int_a^b u'(x)v(x)dx \tag{19}$$

After the first integral on the right hand side is evaluated, we get Equation (16).

Example 3: calculate the indefinite integral of xe^x using integration by parts.

Solution: because the derivative of x is particularly simple and the integral of e^x does not change that function, it makes sense to perform the following procedure

$$\int xe^x dx = \begin{bmatrix} u = x & du = dx \\ dv = e^x dx & v = e^x \end{bmatrix} = xe^x - \int e^x dx = xe^x - e^x + C$$

For definite integrals, the formula for integration by parts retains its limits:

$$\int_a^b \left[u(x)\frac{dv}{dx}\right]dx = u(x)v(x)\Big|_a^b - \int_a^b \left[v(x)\frac{du}{dx}\right]dx \tag{20}$$

where $f(x)\Big|_a^b$ is a shorthand for $f(b)-f(a)$. In practice, the u part is selected to be something that gets simplified by differentiation, and dv is then whatever is left that does not get too complicated after integration. Multiple choices are possible, and practical experience is essential.

Example 4: calculate the integral of $x\cos x$ from 0 to π using integration by parts.

Solution: because the derivative of x is particularly simple and the integral of $\cos x$ is straightforward, it makes sense to perform the following procedure

$$\int_0^\pi x\cos(x)dx = \begin{bmatrix} u = x & du = dx \\ dv = \cos(x)dx & v = \sin(x) \end{bmatrix} = x\sin(x)\Big|_0^\pi - \int_0^\pi \sin(x)dx = [\cdots] = -2$$

3. Integration using recurrence relations

An integral that depends on an integer parameter k can sometimes be reduced to an integral that depends on $k-1$. If the integral with $k=0$ is easy to take, this generates a recurrence relation for the original integral. For example:

$$I_n = \int x^n e^{ax} dx = \begin{Bmatrix} u = x^n & du = nx^{n-1} \\ dv = e^{ax}dx & v = e^{ax}/a \end{Bmatrix} = \frac{x^n e^{ax}}{a} - \frac{n}{a}\int x^{n-1}e^{ax}dx = \frac{x^n e^{ax}}{a} - \frac{n}{a}I_{n-1}$$

In this case I_0 is an easy integral to take and the recurrence relation derived above may then be used to obtain I_n with an arbitrary integer n.

4. Symbolic algebra systems

Purely mathematical research into integration techniques for commonly encountered functions was completed by about 1900. In the context of modern physical sciences, life is too short to integrate manually. Symbolic algebra systems, such as *Mathematica*, are commonly used instead:

```
In[1]:=
        Integrate[1 / (x^4 - a^4), x]
Out[1]=
```

$$-\frac{\text{ArcTan}\left[\frac{x}{a}\right]}{2\,a^3} + \frac{\text{Log}[a-x]}{4\,a^3} - \frac{\text{Log}[a+x]}{4\,a^3}$$

or, for the case of definite integrals:

```
In[2]:=
        Integrate[Sin[x]^2, {x, a, b}]
Out[2]=
        1/2 (-a + b + Cos[a] Sin[a] - Cos[b] Sin[b])
```

Mathematica can take integrals with infinite limits:

```
In[3]:=
        Integrate[1/((2 + x^2) Sqrt[4 + 3 x^2]), {x, -Infinity, Infinity}]
Out[3]=
        ArcCosh[Sqrt[3/2]]
```

as well as integrate very complicated functions, for which the answer is typically returned in terms of highly general functions, such as Meijer G-functions.