CHEM1034 - Week 18 Lecture – Integration, Part I

Chapters 23-25 of Monk and Munro, "Maths for Chemistry", 2nd edition.
Sections 5.1-5.5, 6.1-6.4 of Steiner, "The Chemistry Maths Book", 2nd edition.

Antiderivatives and indefinite integrals

An *antiderivative* of a function $f(x)$ in an interval E is a function $F(x)$ with the following property:

$$F'(x) = f(x) \qquad \forall x \in E \tag{1}$$

The set of all antiderivatives of $f(x)$ in the interval E is called an *indefinite integral* of $f(x)$. Indefinite integrals have the following basic properties:

1. They are defined up to an arbitrary constant:

$$\int f(x)\,dx = F(x) + C \tag{2}$$

2. The derivative of an indefinite integral is the original function:

$$\frac{d}{dx}\int f(x)\,dx = f(x) \tag{3}$$

3. Indefinite integration is a linear operator:

$$\begin{gathered}\int\left[f(x) \pm g(x)\right]dx = \int f(x)\,dx \pm \int g(x)\,dx \\ \int\left[af(x)\right]dx = a\int f(x)\,dx\end{gathered} \tag{4}$$

where a is an arbitrary constant. A table of indefinite integrals may be assembled by constructing functions that have the desired derivatives:

$\frac{df(x)}{dx}$	$f(x)$	$\int f(x)\,dx + C$
nx^{n-1}	x^n	$\frac{1}{n+1}x^{n+1} + C$
e^x	e^x	$e^x + C$
$\frac{1}{x}$	$\ln x$	$x\ln x - x + C$
$-\sin x$	$\cos x$	$\sin x + C$
$\cos x$	$\sin x$	$-\cos x + C$
$-\frac{1}{x^2}$	$\frac{1}{x}$	$\ln x + C$

The task of finding indefinite integrals of functions is not as mechanical as differentiation – there is a theorem that states that a finite algorithm that is able to integrate an arbitrary function does not actually exist. In practice this means that experience and creativity can assist very significantly in the integration process. The following techniques also help:

1. Integration by substitution: let $f(u)$ and $u=\varphi(x)$ be defined in some intervals and let $\varphi(x)$ be differentiable. Then, if $f(u)$ has an antiderivative $F(u)$, then $f(\varphi(x))\varphi'(x)$ has an antiderivative $F(\varphi(x))+C$ and thus

$$\int f(\varphi(x))\varphi'(x)\,dx = F(\varphi(x))+C \tag{5}$$

Proof: using the chain rule to differentiate back the antiderivative

$$\frac{d}{dx}F(\varphi(x)) = \frac{d}{d\varphi}F(\varphi)\frac{d}{dx}\varphi(x) = f(\varphi)\varphi'(x) \tag{6}$$

we can establish that Equation (5) is indeed correct.

Example 1: consider the following integral

$$\int (3x+4)^5\,dx \tag{7}$$

The table above contains no obvious rules that would allow us to integrate this expression. However, we can perform the following substitution:

$$y = 3x+4 \tag{8}$$

computing the differential of this expression provides the connection between dx and dy:

$$dy = 3dx \quad \Rightarrow \quad dx = dy/3 \tag{9}$$

Performing the substitutions in Equation (7) results in the following integral

$$\frac{1}{3}\int y^5 dy \tag{10}$$

which can be taken by using the second line from the table of basic integrals:

$$\frac{1}{3}\int y^5 dy = \frac{1}{18}y^6 + C \tag{11}$$

Using Equation (8) to convert y back into $3x+4$ produces the final answer:

$$\int (3x+4)^5\,dx = \frac{1}{18}(3x+4)^6 + C \tag{12}$$

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

$$\left[\frac{1}{18}(3x+4)^6 + C\right]' = [...] = (3x+4)^5 \tag{13}$$

Example 2: consider the following integral

$$\int x\sqrt{1+x^2}\,dx \tag{14}$$

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:

$$y = 1+x^2 \quad \Rightarrow \quad dy = 2xdx \quad \Rightarrow \quad dx = \frac{dy}{2x} \tag{15}$$

Performing this substitution makes the variable x disappear from the integral

$$\int x\sqrt{1+x^2}\,dx = \int x\sqrt{y}\frac{dy}{2x} = \frac{1}{2}\int y^{1/2}dy \tag{16}$$

This integral is easy to take using the table above:

$$\frac{1}{2}\int y^{1/2}dy=\frac{1}{2}\frac{2}{3}y^{3/2}+C=\frac{1}{3}y^{3/2}+C \tag{17}$$

Back-substitution yields the final answer:

$$\int x\sqrt{1+x^2}\,dx=\frac{1}{3}\left(1+x^2\right)^{3/2}+C \tag{18}$$

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 should be brought back to the original variables after the integration process is finished.

2. Integration by parts: if $u(x)$ and $v(x)$ are differentiable in some interval and their integrals exist, then the following relation holds

$$\int u\,dv=uv-\int v\,du \tag{19}$$

Proof:

$$\begin{gathered} d(uv)=udv+vdu \quad\Rightarrow\quad udv=d(uv)-vdu \quad\Rightarrow \\ \Rightarrow\quad \int udv=\int d(uv)-\int vdu \quad\Rightarrow\quad \int udv=uv-\int vdu \end{gathered} \tag{20}$$

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

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

Definite integrals

Let $[a,b]$ be a closed interval on the real line, let the set of sub-intervals

$$\left\{[x_0,x_1],[x_1,x_2],\ldots,[x_{n-1},x_n]\right\} \tag{21}$$

be a partition of that interval, such that

$$a=x_0<x_1<x_2<\ldots<x_n=b \tag{22}$$

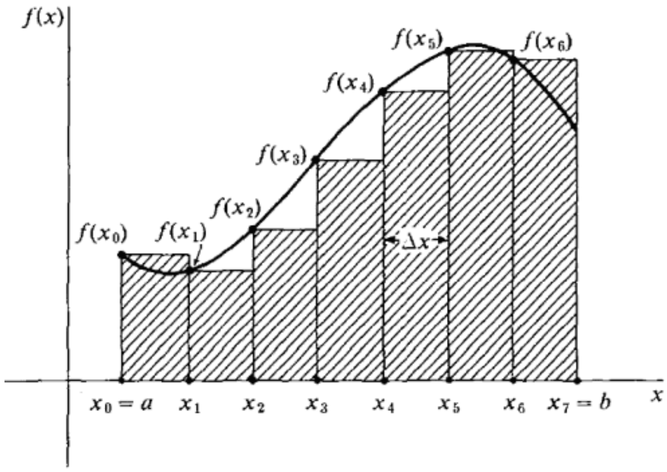
and let $\xi_k\in[x_k,x_{k+1}]$ be points arbitrarily chosen within those intervals.

A function $f(x)$ is called *Riemann integrable* on the interval $[a,b]$ if, for any sequence of partitions in which the size of the sub-intervals is gradually reduced, the following limit exists:

$$\lim_{n\to\infty}\sum_{k=0}^{n-1} f(\xi_k)\Delta x_k \tag{23}$$

The value of this limit is called the Riemann integral of $f(x)$ on the interval $[a,b]$ and denoted

$$\int_a^b f(x)\,dx \tag{24}$$



In many cases the definite integral may be interpreted as the area under the function graph. The Riemann definition of the definite integral is used by numerical algorithms in modern computers. The best analytical way of computing definite integrals is to use the Newton-Leibnitz formula, which will be given here without proof:

$$\int_a^b f(x)dx = F(b) - F(a) \tag{25}$$

where $F(b)$ and $F(a)$ are values of the *indefinite integral* of the function $f(x)$ at the integration limits (the constant cancels). The limit definition in Equation (23) may be used, but is in practice rather inconvenient.

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:

$$\int_a^b f(x)dx = \int_{u(a)}^{u(b)} \left[f(u)\left(\frac{du}{dx}\right)^{-1} \right] du \tag{26}$$

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

Solution: the integral in question would become much simpler if $u = 4x+5$:

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

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

The formula for integration by parts also acquires limits:

$$\int_a^b \left[u(x)\frac{dv}{dx} \right] dx = u(x)v(x)\Big|_a^b - \int_a^b \left[v(x)\frac{du}{dx} \right] dx \tag{27}$$

where $f(x)\big|_a^b$ is a shorthand for $f(b) - f(a)$.

Week 19 workshop exercises

Monk and Munro, 2nd edition: Chapter 23, self-tests 23.1, 23.2, 23.3; problems 23.1-23.10; Chapter 24, self-tests 24.1, 24.2; problems 24.1-24-10.

The table and the integration exercises below come from the very famous book that was the standard mathematics problem set for all Chemistry undergraduates in ex-USSR.

Extended table of indefinite integrals

I. $\int x^n dx = \frac{x^{n+1}}{n+1} + C, \quad n \neq -1.$

II. $\int \frac{dx}{x} = \ln|x| + C.$

III. $\int \frac{dx}{x^2+a^2} = \frac{1}{a} \operatorname{artan} \frac{x}{a} + C = -\frac{1}{a} \operatorname{arcot} \frac{x}{a} + C \quad (a \neq 0).$

IV. $\int \frac{dx}{x^2-a^2} = \frac{1}{2a} \ln\left|\frac{x-a}{x+a}\right| + C \quad (a \neq 0).$

$\int \frac{dx}{a^2-x^2} = \frac{1}{2a} \ln\left|\frac{a+x}{a-x}\right| + C \quad (a \neq 0).$

V. $\int \frac{dx}{\sqrt{x^2+a}} = \ln\left|x + \sqrt{x^2+a}\right| + C \quad (a \neq 0).$

VI. $\int \frac{dx}{\sqrt{a^2-x^2}} = \operatorname{arsin} \frac{x}{a} + C = -\operatorname{arcos} \frac{x}{a} + C \quad (a > 0).$

VII. $\int a^x dx = \frac{a^x}{\ln a} + C \quad (a > 0); \quad \int e^x dx = e^x + C.$

VIII. $\int \sin x \, dx = -\cos x + C.$

IX. $\int \cos x \, dx = \sin x + C.$

X. $\int \frac{dx}{\cos^2 x} = \tan x + C.$

XI. $\int \frac{dx}{\sin^2 x} = -\cot x + C.$

XII. $\int \frac{dx}{\sin x} = \ln\left|\tan \frac{x}{2}\right| + C = \ln|\operatorname{cosec} x - \cot x| + C.$

XIII. $\int \frac{dx}{\cos x} = \ln\left|\tan\left(\frac{x}{2} + \frac{\pi}{4}\right)\right| + C = \ln|\tan x + \sec x| + C.$

XIV. $\int \sinh x \, dx = \cosh x + C.$

XV. $\int \cosh x \, dx = \sinh x + C.$

XVI. $\int \frac{dx}{\cosh^2 x} = \tanh x + C.$

XVII. $\int \frac{dx}{\sinh^2 x} = -\coth x + C.$

Extra difficulty exercises for the brave

1031. $\int 5a^2x^6dx.$

1032. $\int (6x^2+8x+3)\,dx.$

1033. $\int x(x+a)(x+b)\,dx.$

1034. $\int (a+bx^3)^2\,dx.$

1035. $\int \sqrt{2px}\,dx.$

1036. $\int \frac{dx}{\sqrt[n]{x}}.$

1037. $\int (nx)^{\frac{1-n}{n}}\,dx.$

1038. $\int \left(a^{\frac{2}{3}}-x^{\frac{2}{3}}\right)^3 dx.$

1039. $\int (\sqrt{x}+1)(x-\sqrt{x}+1)\,dx.$

1040. $\int \frac{(x^2+1)(x^2-2)}{\sqrt[3]{x^2}}\,dx.$

1041. $\int \frac{(x^m-x^n)^2}{\sqrt{x}}\,dx.$

1042. $\int \frac{(\sqrt{a}-\sqrt{x})^4}{\sqrt{ax}}\,dx.$

1043. $\int \frac{dx}{x^2+7}.$

1044. $\int \frac{dx}{x^2-10}.$

1045. $\int \frac{dx}{\sqrt{4+x^2}}.$

1046. $\int \frac{dx}{\sqrt{8-x^2}}.$

1047. $\int \frac{\sqrt{2+x^2}-\sqrt{2-x^2}}{\sqrt{4-x^4}}\,dx.$

1051**. $\int \frac{a\,dx}{a-x}.$

1052**. $\int \frac{2x+3}{2x+1}\,dx.$

1053. $\int \frac{1-3x}{3+2x}\,dx.$

1054. $\int \frac{x\,dx}{a+bx}.$

1055. $\int \frac{ax+b}{\alpha x+\beta}\,dx.$

1056. $\int \frac{x^2+1}{x-1}\,dx.$

1057. $\int \frac{x^2+5x+7}{x+3}\,dx.$

1058. $\int \frac{x^4+x^2+1}{x-1}\,dx.$