CHEM1047 - Week 9 Lecture 1 - Definition of a function integral

☐ *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.*

1. Antiderivative and indefinite integral

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 the *indefinite integral* of $f(x)$. Indefinite integrals have the following basic properties:

1. They are defined up to an arbitrary constant:

$$\left[F(x)+c\right]' = f(x) \qquad \forall c \in \mathbb{C} \tag{2}$$

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:

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

where α is an arbitrary scalar.

2. Riemann integral

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

$$\left\{[x_0,x_1],[x_1,x_2],\ldots,[x_{n-1},x_n]\right\} \tag{5}$$

be a partition of that interval, such that

$$a = x_0 < x_1 < x_2 < \ldots < x_n = b, \tag{6}$$

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

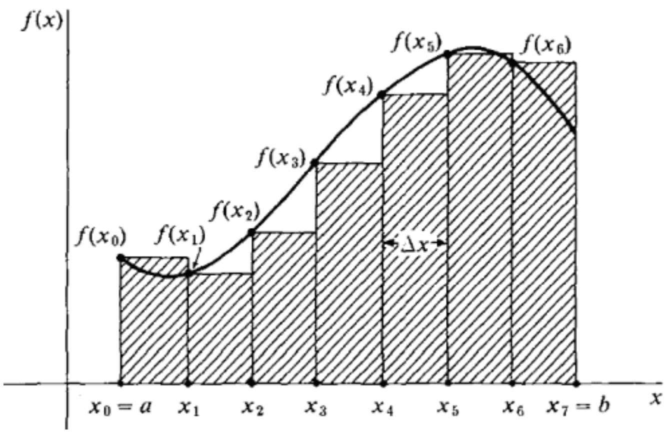

Figure 1. Graphical illustration of Equations (5) and (6), showing a partitioning of the interval [a,b] with seven sub-intervals. The function value is taken at the leftmost point of each interval.

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:

$$\lim_{n\to\infty}\sum_{k=0}^{n-1} f(\xi_k)\Delta x_k \tag{7}$$

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

$$\int_a^b f(x)\,dx \tag{8}$$

The definite integral may be interpreted as the area under the function graph. Examples of integrable functions are polynomials for which the limit in Equation (7) always exists. Non Riemann integrable functions either have singularities within the integration interval (for example, $f(x)=1/x$), or the value of the function does not stop changing from one point to the next (*e.g.* Dirichlet function).

Some important properties of Riemann integrals are:

1. *Concatenation*:

$$\int_a^{b+c} f(x)\,dx = \int_a^b f(x)\,dx + \int_b^c f(x)\,dx \tag{9}$$

when $f(x)$ is integrable in all of the intervals involved.

2. *Mean value theorem*:

$$\int_a^b f(x)\,dx = (b-a)\,f(c) \tag{10}$$

for a continuous function $f(x)$ where $c\in[a,b]$. This is illustrated in Figure 2 below.

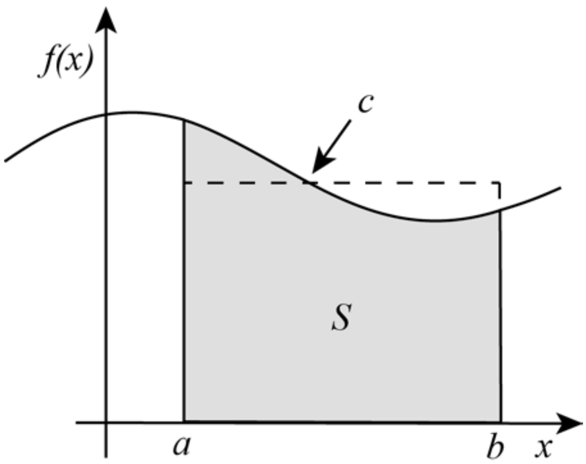

Figure 2. A graphical illustration of the mean value theorem in Equation (10).

3. *Limit inversion* and *identical limits*:

$$\int_a^b f(x)\,dx = -\int_b^a f(x)\,dx, \qquad \int_a^a f(x)\,dx = 0 \tag{11}$$

The minus appears in the first integral because the signs of Δx_k in Equation (7) flip. The second integral is equal to zero because all $\Delta x_k = 0$ when the limits are equal.

3. Newton-Leibniz formula

There is an obvious missing link between the indefinite integral in Equation (2), which is essentially inverse differentiation, and the limit in Equation (7), which may be interpreted as the area under the graph. The connection is provided by a corollary to the theorem that we will now prove.

Theorem ("*first fundamental theorem of calculus*"): let $f(x)$ be a continuous and Riemann integrable function defined on a closed interval $[a,b]$, and let $F(x)$ be defined for all $x \in [a,b]$ as

$$F(x) = \int_a^x f(t)\,dt \qquad (12)$$

Then $F(x)$ is an antiderivative of $f(x)$ for all $x \in (a,b)$.

Proof (examinable): consider a point $x \in (a,b)$ and an increment Δx chosen so that $x + \Delta x \in (a,b)$. The difference between the values of F at those points follows from the definition in Equation (12):

$$F(x+\Delta x) - F(x) = \int_a^{x+\Delta x} f(t)\,dt - \int_a^x f(t)\,dt$$

However, from the combination property in Equation (9):

$$\int_a^{x+\Delta x} f(t)\,dt = \int_a^x f(t)\,dt + \int_x^{x+\Delta x} f(t)\,dt$$

and therefore:

$$F(x+\Delta x) - F(x) = \int_x^{x+\Delta x} f(t)\,dt$$

We can further simplify the integral using the mean value theorem in Equation (10):

$$\int_x^{x+\Delta x} f(t)\,dt = f(c)\Delta x, \qquad c \in [x, x+\Delta x]$$

After dividing both sides by Δx, we obtain:

$$\frac{F(x+\Delta x) - F(x)}{\Delta x} = f(c)$$

Finally, we will take the limit of $\Delta x \to 0$. Note that c is positioned between x and $x + \Delta x$, and therefore driven to $c = x$. We therefore obtain:

$$\lim_{\Delta x \to 0} \frac{F(x+\Delta x) - F(x)}{\Delta x} = \lim_{\Delta x \to 0} f(c) \qquad \Rightarrow \qquad F'(x) = f(x)$$

as required. Therefore, $F(x)$ defined in Equation (12) is indeed an antiderivative of $f(x)$.

Corollary (*Newton-Leibniz formula*):

$$\int_\alpha^\beta f(x)\,dx = F(\beta) - F(\alpha) \qquad (13)$$

where $\alpha \in [a,b]$, $\beta \in [a,b]$, and $F(x)$ is an antiderivative of $f(x)$.

Proof (examinable): using Equation (12) for the antiderivative and the concatenation rule,

$$F(\beta)-F(\alpha)=\int_{a}^{\beta} f(t)\,dt-\int_{a}^{\alpha} f(t)\,dt=\int_{a}^{\beta} f(t)\,dt+\int_{\alpha}^{a} f(t)\,dt=\int_{\alpha}^{\beta} f(t)\,dt$$

which is exactly the same as Equation (13).