THE CHEMIST'S TOOLKIT 5 Differentiation

Differentiation is concerned with the slopes of functions, such as the rate of change of a variable with time. The formal definition of the **derivative**, $\mathrm{d}f/\mathrm{d}x$, of a function $f(x)$ is

$$\frac{\mathrm{d}f}{\mathrm{d}x}=\lim_{\delta x\to 0}\frac{f(x+\delta x)-f(x)}{\delta x} \qquad \text{First derivative [definition]} \qquad (5.1)$$

As shown in Sketch 5.1, the derivative can be interpreted as the slope of the tangent to the graph of $f(x)$ at a given value of x. A positive first derivative indicates that the function slopes upwards (as x increases), and a negative first derivative indicates the opposite. It is sometimes convenient to denote the first derivative as $f'(x)$. The **second derivative**, $\mathrm{d}^2f/\mathrm{d}x^2$, of a function is the derivative of the first derivative (here denoted f'):

$$\frac{\mathrm{d}^2f}{\mathrm{d}x^2}=\lim_{\delta x\to 0}\frac{f'(x+\delta x)-f'(x)}{\delta x} \qquad \text{Second derivative [definition]} \qquad (5.2)$$

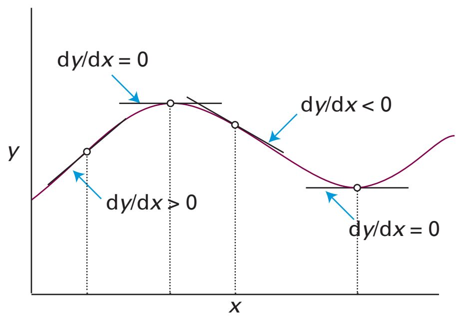
It is sometimes convenient to denote the second derivative f''. As shown in Sketch 5.2, the second derivative of a function can be interpreted as an indication of the sharpness of the curvature of the function. A positive second derivative indicates that the function is ∪ shaped, and a negative second derivative indicates that it is ∩ shaped. The second derivative is zero at a **point of inflection**, where the first derivative passes through zero but does not change sign.

The derivatives of some common functions are as follows:

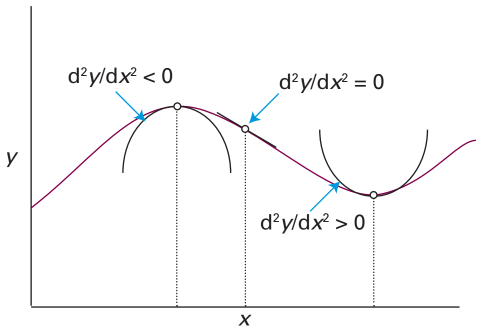
$$\frac{\mathrm{d}}{\mathrm{d}x}x^n=nx^{n-1}$$

$$\frac{\mathrm{d}}{\mathrm{d}x}\mathrm{e}^{ax}=a\mathrm{e}^{ax}$$

$$\frac{\mathrm{d}}{\mathrm{d}x}\sin ax=a\cos ax \qquad \frac{\mathrm{d}}{\mathrm{d}x}\cos ax=-a\sin ax$$



Sketch 5.1



Sketch 5.2

$$\frac{\mathrm{d}}{\mathrm{d}x}\ln ax=\frac{1}{x}$$

It follows from the definition of the derivative that a variety of combinations of functions can be differentiated by using the following rules:

$$\frac{\mathrm{d}}{\mathrm{d}x}(u+v)=\frac{\mathrm{d}u}{\mathrm{d}x}+\frac{\mathrm{d}v}{\mathrm{d}x}$$

$$\frac{\mathrm{d}}{\mathrm{d}x}uv=u\frac{\mathrm{d}v}{\mathrm{d}x}+v\frac{\mathrm{d}u}{\mathrm{d}x}$$

$$\frac{\mathrm{d}}{\mathrm{d}x}\frac{u}{v}=\frac{1}{v}\frac{\mathrm{d}u}{\mathrm{d}x}-\frac{u}{v^2}\frac{\mathrm{d}v}{\mathrm{d}x}$$

Brief illustration 5.1: Derivatives of a product of functions

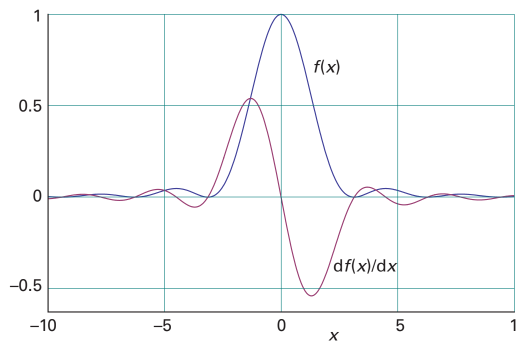
To differentiate the function $f=\sin^2 ax/x^2$ write

$$\frac{\mathrm{d}}{\mathrm{d}x}\frac{\sin^2 ax}{x^2}=\frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{\sin ax}{x}\right)\left(\frac{\sin ax}{x}\right)=2\left(\frac{\sin ax}{x}\right)\frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{\sin ax}{x}\right)$$

$$=2\left(\frac{\sin ax}{x}\right)\left\{\frac{1}{x}\frac{\mathrm{d}}{\mathrm{d}x}\sin ax+\sin ax\frac{\mathrm{d}}{\mathrm{d}x}\frac{1}{x}\right\}$$

$$=2\left\{\frac{a}{x^2}\sin ax\cos ax-\frac{\sin^2 ax}{x^3}\right\}$$

The function and this first derivative are plotted in Sketch 5.3.



Sketch 5.3

It is sometimes convenient to differentiate with respect to a function of x, rather than x itself.

Brief illustration 5.2: Differentiation with respect to a function

Suppose that

$$f(x)=a+\frac{b}{x}+\frac{c}{x^2}$$

where a, b, and c are constants and you need to evaluate $\mathrm{d}f/\mathrm{d}(1/x)$, rather than $\mathrm{d}f/\mathrm{d}x$. To begin, let $y=1/x$. Then $f(y)=a+by+cy^2$ and

$$\frac{\mathrm{d}f}{\mathrm{d}y}=b+2cy$$

Because $y=1/x$, it follows that

$$\frac{\mathrm{d}f}{\mathrm{d}(1/x)}=b+\frac{2c}{x}$$