The chemist's toolkit 4 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

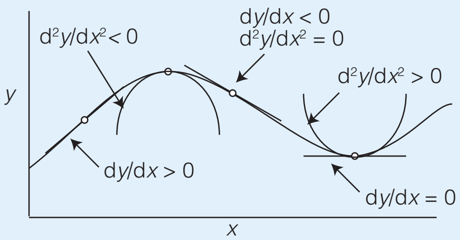
$$\frac{\mathrm{d}f}{\mathrm{d}x}=\lim_{\delta x\to 0}\frac{f(x+\delta x)-f(x)}{\delta x}$$ First derivative [definition]

As shown in the sketch, a derivative can be interpreted as the slope of the tangent to the graph of $f(x)$. 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'):

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

It is sometimes convenient to denote the second derivative $f''(x)$. As shown in the sketch, 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 derivatives of some common functions (with a a constant) are as follows:

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

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

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

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

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

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

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

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

A function of the form $f(x,y)$ depends on two variables. To take its derivative, one of the variables, x or y, is held constant and the slope of the function with respect to the other variable is the **partial derivative** of the function. A partial derivative is denoted

$$\left(\frac{\partial f}{\partial x}\right)_y \quad \text{or} \quad \left(\frac{\partial f}{\partial y}\right)_x$$

The subscript expresses which of the variables is held constant. The symbol ∂ is commonly read as 'curly dee'.