The chemist's toolkit 7 Series expansions

A function $f(x)$ can be expressed in terms of its value in the vicinity of $x = a$ by using the **Taylor series**

$$f(x) = f(a) + \left(\frac{df}{dx}\right)_a (x-a) + \frac{1}{2!}\left(\frac{d^2f}{dx^2}\right)_a (x-a)^2 + \cdots$$ Taylor series

where the notation $(\ldots)_a$ means that the derivative is evaluated at $x = a$ and $n!$ denotes a **factorial** defined as

$$n! = n(n-1)(n-2)\ldots 1, \qquad 0! \equiv 1$$ Factorial

The **Maclaurin series** for a function is a special case of the Taylor series in which $a = 0$. The following Maclaurin series are used at various stages in the text:

$$(1+x)^{-1} = 1 - x + x^2 - \cdots$$

$$e^x = 1 + x + \tfrac{1}{2}x^2 + \cdots$$

$$\ln(1+x) = x - \tfrac{1}{2}x^2 + \tfrac{1}{3}x^3 - \cdots$$

Series expansions are used to simplify calculations, because when $|x| << 1$ it is possible, to a good approximation, to terminate the series after one or two terms. Thus, provided $|x| << 1$,

$$(1+x)^{-1} \approx 1 - x$$

$$e^x \approx 1 + x$$

$$\ln(1+x) \approx x$$

A series is said to **converge** if the sum approaches a finite, definite value as n approaches infinity. If it does not, the series is said to **diverge**. Thus, the series expansion of $(1+x)^{-1}$ converges for $|x| < 1$ and diverges for $|x| \geq 1$. Tests for convergence are explained in mathematical texts.