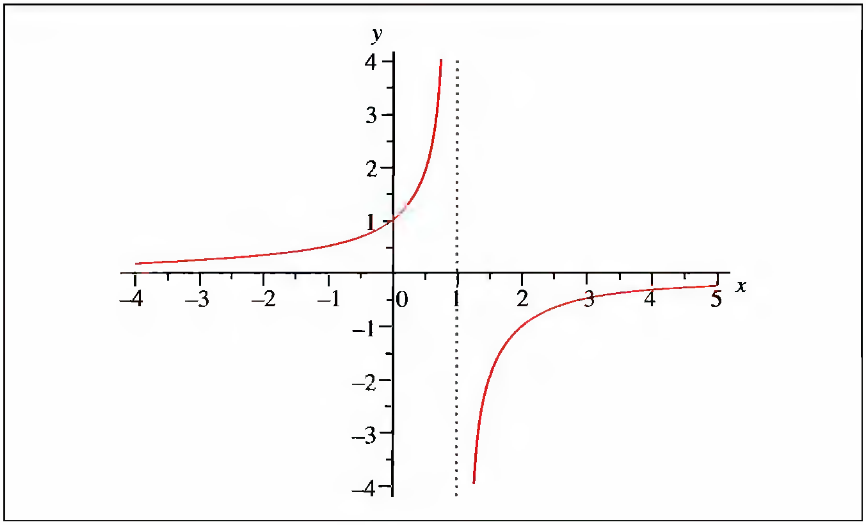

Figure 3.2 A plot of the function $f(x) = 1/(1 - x)$

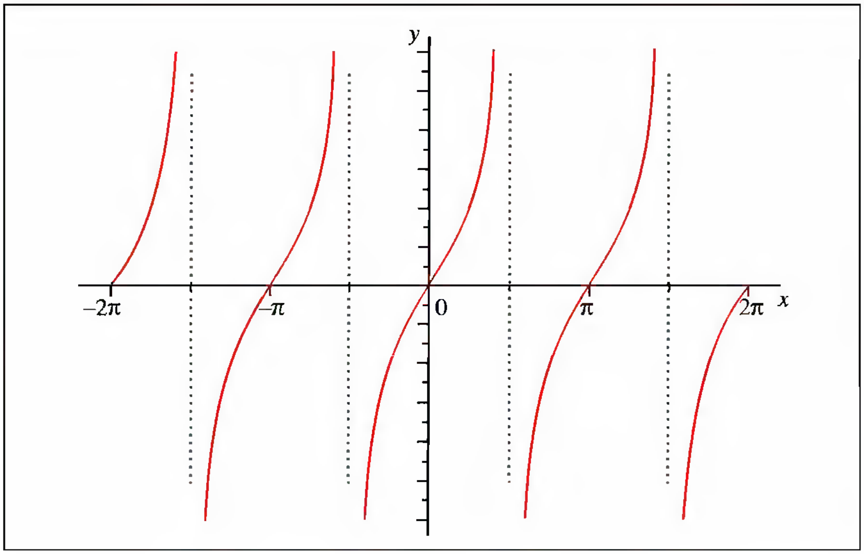

Figure 3.3 A plot of the function $f(x) = \tan x$

3.1.2 Limiting Behaviour for Increasingly Large Positive or Negative Values of the Independent Variable

We now turn to examining the limiting behaviour of functions as the independent variable takes on increasingly large positive or negative values. As an illustration, consider the function shown in Figure 3.2. We see from the form of $f(x)$ that the value of y approaches zero as x becomes increasingly large in both positive and negative senses: the line $y = 0$ is an asymptote. In the former case the values of y are increasingly small negative numbers and in the latter they are increasingly small positive numbers. The **limiting values** of $f(x)$ are therefore zero in both cases.

Periodic functions such as sin x or cos x have no asymptotes (no single limiting value), because their values oscillate between two limits as the independent variable increases in a positive or negative sense. For example, the value of the function $f(x) = \cos(2x)$ oscillates between $+1$ and -1 as $x \to \infty$ (see Figure 3.4).

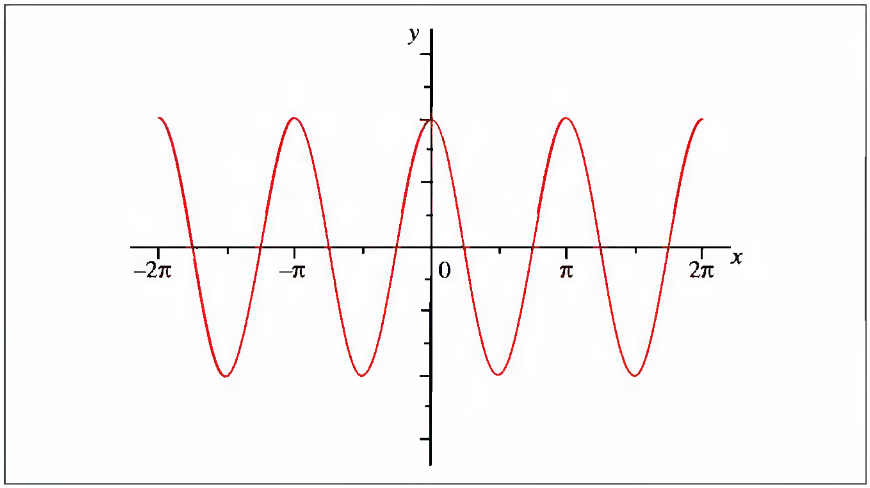

Figure 3.4 A plot of the function $f(x) = \cos(2x)$

Problem 3.1

Find the limiting values for (a) x^2e^{-x} and (b) $\cos(2x)e^{-x}$ as $x \to \infty$.

3.1.3 Limiting Behaviour for Increasingly Small Values of the Independent Variable

Frequently, the context of a particular problem requires us to consider the limiting behaviour of a function as the value of the independent variable approaches zero. For example, consider the physical measurement of heat capacity at absolute zero. Since it is impossible to achieve absolute zero in the laboratory, a natural way to approach the problem would be to obtain measurements of the property at increasingly lower temperatures. If, as the temperature is reduced, the corresponding measurements approach some value m, then it may be assumed that the measurement of the property (in this case, heat capacity) at absolute zero is also m, so long as the specific heat function is continuous in the region of study. We say in this case that the limiting value of the heat capacity, as the temperature approaches absolute zero, is m. As we shall see in Section 3.2, the notation we use to describe this behaviour is:

$$\lim_{T \to 0} C_V(T) = m \tag{3.1}$$

where, in this case, $m = 0$ because the limiting value of the heat capacity as $T \to 0$ K is zero. It is also important to note that it is only possible to approach absolute zero from positive values of T; thus, in this situation, the "right" limit, usually written as $\lim_{T \to 0^+} C_V(T) = m$, is the only one of physical significance.

Problem 3.2

Find the limiting values for (a) x^2e^{-x} and (b) $\cos(2x)e^{-x}$ as $x \to 0$.

3.2 Defining the Limiting Process

For a function of a single variable x, symbolized, as usual, by $y = f(x)$, we are interested in the value of $f(x)$ as x approaches a particular value, a, but never takes the value a. Points where the function is not defined, as seen, for example, at $x = 1$ in Figure 3.2, are excluded from the domain of the function; at other points, the function is continuous.

Limits play an important role in probing the behaviour of a function at any point in its domain, and the notation we use to describe this process is:

$$\lim_{x \to a} f(x) = m \tag{3.2}$$

Note: in this symbolism, the suffix to the symbol lim indicates that, although x approaches a, it *never* actually takes the value a. For the limit to exist, the same (finite) result must be obtained whether we approach a from smaller or larger values of x. Furthermore, if $m = f(a)$, then the function is said to be continuous at $x = a$.

3.2.1 Finding the Limit Intuitively

Consider the plot of the function:

$$y = f(x), \text{ where } f(x) = \frac{x^2 - 9}{x - 3} \tag{3.3}$$

shown in Figure 3.1. It is evident that $f(x)$ is continuous (unbroken) for all values of x except $x = 3$. Since the denominator and numerator of the function are both zero at $x=3$, we see that the function is indeterminate at this value of x; however, as seen in Table 3.1, the *ratio* of the numerator and denominator seems to be approaching the value $y=6$ as $x \to 3$ from smaller or larger values.

Table 3.1 Values of $f(x) = (x^2-9)/(x-3)$ in the vicinity of $x=3$

x	x^2-9	$x-3$	$(x^2-9)/(x-3)$
4	7	1	7
3.5	3.25	0.5	6.5
3.1	0.61	0.1	6.1
3.01	0.0601	0.01	6.01
3	0	0	indeterminate
2.99	−0.0599	−0.01	5.99
2.9	−0.59	−0.1	5.9
2.5	−2.75	−0.5	5.5
2	−5	−1	5

Taking even smaller increments either side of 3, say $x=3 \pm 0.0001$, we find that $f(3.0001)=6.0001$ and $f(2.9999)=5.9999$. These results suggest that for smaller and smaller increments in x, either side of $x=3$, the values of the function become closer and closer to 6. Thus we say that, in the limit as $x \to 3$, m takes the value 6:

$$\lim_{x\to 3} \frac{x^2-9}{x-3} = 6 \tag{3.4}$$

3.2.2 An Algebraic Method for Evaluating Limits

In practice, it is often easiest when evaluating limits to write $x=a \pm \delta$, and consider what happens as $\delta \to 0$, *but never takes the value zero*. This procedure allows us to let x become as close as we like to the value a, *without* it taking the value $x=a$.

Worked Problem 3.1

Q Evaluate $\lim_{x\to 3} f(x)$, where $f(x) = \dfrac{x^2-9}{x-3}$.

A By substituting $x=3+\delta$ in the expression for $f(x)$, and expanding the square term in the numerator, we obtain:

$$\lim_{x\to 3} \frac{x^2-9}{x-3} = \lim_{\delta\to 0} \frac{(3+\delta)^2-9}{3+\delta-3}$$

$$= \lim_{\delta \to 0} \frac{9 + 6\delta + \delta^2 - 9}{\delta} = \lim_{\delta \to 0} \frac{6\delta + \delta^2}{\delta}$$

$$= \frac{6 - \delta}{1} = 6$$

where, in the last step, δ can be cancelled in every term of the numerator and denominator as its value is never zero. Thus we obtain the expected result that $f(x)$ approaches the limiting value of 6 as x tends to the value 3, irrespective of the sign of δ. In this situation, m in the definition of the limit has the value 6.

Problem 3.3

For each of the following functions, $f(x)$, identify any points of discontinuity (those values of x where the function is of indeterminate value) and use the method described in Worked Problem 3.1, where appropriate, to find the limiting values of the following functions at your suggested points of discontinuity.

(a) $f(x) = \frac{2x}{x-4}$; (b) $f(x) = \frac{x^2 - 4}{x - 2}$; (c) $f(x) = \frac{x - 1}{x^2 - 1}$;

(d) $f(x) = 3x^2 - \frac{2}{x} - 1$.

3.2.3 Evaluating Limits for Functions whose Values become Indeterminate

Whenever the value of a function becomes indeterminate for particular limiting values in the independent variable (for example, division by zero or expressions such as ∞/∞ or $\infty - \infty$), we need to adopt alternative strategies in determining the limiting behaviour. Such situations arise quite commonly in chemistry, especially when we are interested in evaluating some quantity as the independent variable takes on increasingly large or small values. Good examples occur in dealing with mathematical expressions arising in:

- Manipulating the solutions of rate equations in kinetics.
- Determining high- or low-temperature limits of thermodynamic properties.

Worked Problem 3.2

Q Find $\lim_{x\to\infty} \frac{2x^2+4}{x^2-x+1}$.

A Both the numerator and denominator tend to infinity as $x \to \infty$, but their ratio remains finite. There are two ways of handling this situation:

First, we note that as x becomes very large, $2x^2+4$ is increasingly well approximated by $2x^2$, and x^2-x+1 by x^2 as, in both expressions, the highest power of x dominates as x becomes indefinitely large. Thus, as x increases without limit, we find:

$$\lim_{x\to\infty} \frac{2x^2+4}{x^2-x+1} = \lim_{x\to\infty} \frac{2x^2}{x^2} = \lim_{x\to\infty} 2 = 2$$

Second, we could divide the numerator and denominator by the highest power of x, before taking the limit:

$$\lim_{x\to\infty} \frac{2x^2+4}{x^2-x+1} = \lim_{x\to\infty} \frac{2+4/x^2}{1-1/x+1/x^2} = 2$$

and, again, we see that as x increases without limit, the ratio of numerator to denominator tends to 2.

Problem 3.4

Evaluate the following limits:

(a) $\lim_{x\to\infty} \frac{5}{x+1}$; (b) $\lim_{x\to\infty} \frac{3x}{x-4}$; (c) $\lim_{x\to\infty} \frac{x^2}{x+1}$; (d) $\lim_{x\to\infty} \frac{x+1}{x+2}$.

The limiting behaviour of functions for increasingly small values of the independent variable can be found in a similar way by applying exactly the same principles, except that, now, the lowest power of x provides the largest term in both numerator and denominator.

Worked Problem 3.3

Q Find $\lim_{x\to 0} \frac{x^2+x}{x^3-1}$.

A This time, for increasingly small values of x, the numerator and denominator are dominated by x and -1, respectively. Consequently, the ratio of the numerator to denominator tends to $\frac{x}{-1}$, which leads to a limiting value of zero: $\lim_{x\to 0} \frac{x}{-1} = 0$.

Problem 3.5

Evaluate the limit $\lim_{x \to 0}(\ln x - \ln 2x)$.
Hint: remember that $\ln a - \ln b = \ln \frac{a}{b}$ (see Chapter 2).

Problem 3.6

The Einstein model for the molar heat capacity of a solid at constant volume, C_V, yields the formula:

$$C_V = 3R(ax)^2 \left\{ \frac{e^{ax/2}}{e^{ax} - 1} \right\}^2$$

where $a = \frac{h\nu}{k}$ and $x = \frac{1}{T}$. Find the limiting value of C_V as $T \to 0$ K, remembering that $x = \frac{1}{T}$.

Note: we shall revisit this problem in Chapter 1 of Volume 2, where we explore the limiting behaviour for high values of T (Problem 1.10, Volume 2).

Problem 3.7

The radial function for the 3s atomic orbital of the hydrogen atom has the form:

$$R_{3s} = N\left(\frac{r}{a_0}\right)^2 e^{-r/a_0}$$

where N is a constant. Find the values of R_{3s} as: (a) $r \to 0$; (b) $r \to \infty$.
Hint: see your answers to Problems 3.1(a) and 3.2(a).

3.2.4 The Limiting Form of Functions of More Than One Variable

Sometimes, we are interested in how the form of a function might change for limiting values in one or more variables. For example, consider the catalytic conversion of sucrose to fructose and glucose by the enzyme invertase (β-fructofuranidase). The rate of formation of product P for this reaction varies in a rather complicated way with the sucrose concentration [S]. At low [S], the reaction is first order in [S], and at high [S] it is zero order. The behaviour observed in Figure 3.5 is established by investigating the form of the function describing the rate of reaction for the two limiting cases where [S] approaches either very large or very small values, rather than the absolute value of the function as in the examples discussed above. This is a consequence in this case of the rate equation being a function of more than one variable.

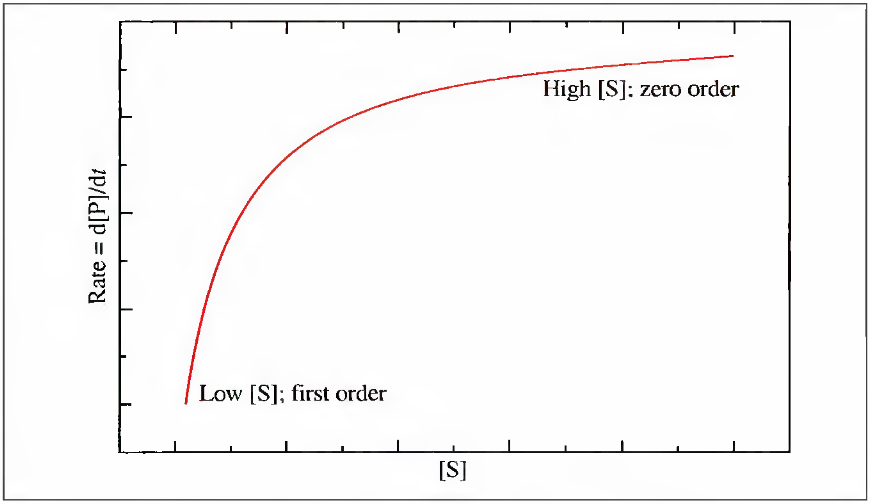

Figure 3.5 The variation in rate of enzymolysis for low and high sucrose concentration, [S], where the reaction is first and zero order, respectively

Worked Problem 3.4

Q The rate of formation of the product P in the catalytic conversion of sucrose to fructose and glucose by the enzyme invertase is given by:

$$\frac{d[P]}{dt} = \frac{k_2[E]_0[S]}{K_M + [S]}$$

where k_2 is a rate constant, K_M is known as the Michaelis constant, $[E]_0$ is the initial enzyme concentration and [S] is the sucrose concentration. Find the order of reaction with respect to [S] when (a) $[S] \gg K_M$ and (b) $[S] \ll K_M$.

A (a) For $[S] \gg K_M$, $K_M + [S] \approx [S]$ and so $\frac{d[P]}{dt} = \frac{k_2[E]_0[S]}{K_M + [S]} \approx \frac{k_2[E]_0[S]}{[S]} = k_2[E]_0$: zero order in [S].

(b) For $[S] \ll K_M$, $K_M + [S] \approx K_M$ and $\frac{d[P]}{dt} = \frac{k_2[E]_0[S]}{K_M + [S]} \approx \frac{k_2[E]_0[S]}{K_M}$: first order in [S].

Problem 3.8

A rate law derived from a steady-state analysis of a reaction mechanism proposed for the reaction of H_2 with NO is given by:

$$\frac{d[N_2]}{dt} = \frac{k_1 k_2 [H_2][NO]^2}{k_{-1} + k_2[H_2]}$$

Find the limiting form of the rate law when (a) $k_{-1} \gg k_2[H_2]$ and (b) $k_{-1} \ll k_2[H_2]$.

Summary of Key Points

This chapter introduces the concept of the limit, with a view not only to probing limiting behaviour of functions but also as a foundation to the development of differential and integral calculus in the following chapters. The key points discussed include:

1. The principles involved and notation used in defining a limit.

2. Point discontinuities, infinite discontinuities and asymptotic behaviour.

3. Finding a limit intuitively and algebraically.

4. Investigating the limiting value of functions for increasingly large and small values of the independent variable.

5. Finding the limiting forms of functions of more than one variable.

4
Differentiation

A great deal of chemistry is concerned with processes in which properties change as a function of some variable. Good examples are found in the field of chemical kinetics, which is concerned with measuring and interpreting changes in concentrations of reactants or products with time, and in quantum mechanics, where we are interested in the rate of change in the electronic wavefunction of a diatomic molecule as a function of bond length.

Aims

Calculus is of fundamental importance in chemistry because it underpins so many key chemical concepts. In this chapter, we discuss the foundations and applications of **differential calculus**; by the end of the chapter you should be able to:

- Describe processes involving change in one independent variable
- Define the average rate of change of the dependent variable
- Use the concepts of limits to define the instantaneous rate of change
- Differentiate most of the standard mathematical functions by rule
- Differentiate a sum, product or quotient of functions
- Apply the chain rule to non-standard functions
- Understand the significance of higher-order derivatives and identify maxima, minima and points of inflection
- Understand the concept of the differential operator
- Understand the basis of the eigenvalue problem and identify eigenfunctions, eigenvalues and operators
- Differentiate functions of more than one variable

4.1 The Average Rate of Change

Consider the plot of the function $y = f(x)$, in which x is the independent variable, shown in Figure 4.1. The **average rate of change** of $f(x)$ over the increment Δx in x is given by:

$$\frac{QR}{PR} = \frac{f(x_0 + \Delta x) - f(x_0)}{\Delta x} = \frac{\Delta y}{\Delta x} \tag{4.1}$$

where $f(x_0)$ and $f(x_0 + \Delta x)$ are the values of $f(x)$ at the points x_0 and $x_0 + \Delta x$, and Δy is the change in y that results in the change Δx in x.

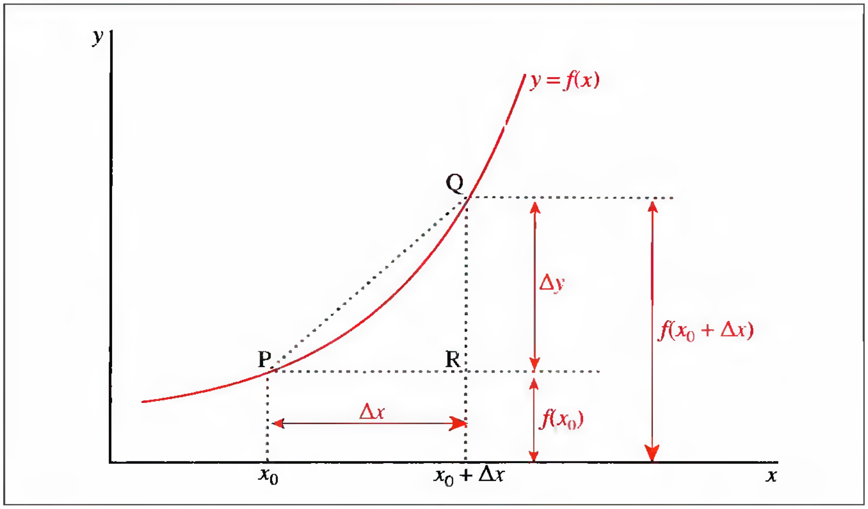

Figure 4.1 Defining the average rate of change of $f(x)$ as x is incremented from x_0 to $x_0 + \Delta x$

This average rate of change corresponds to the slope of the **chord** PQ; that is, the slope of the straight line (sometimes termed the **secant**) joining P and Q. In chemical kinetics, we can draw a direct analogy by equating the concentration of a species A at time t, often designated by [A], to the dependent variable (designated as y in Figure 4.1), and the time after initiation of the reaction, t, to the independent variable (designated by x in Figure 4.1). Consequently, if we measure the concentration of a reaction product at two intervals of time, say one minute apart, we might conclude that over that interval the concentration of the product had changed by 1.00 mol dm^{-3}. In this case, we could state that the average rate of reaction in this interval is 1.00 mol dm^{-3} per minute. The problem here is that we know nothing about how the reaction rate changes in detail during that interval of one minute, and it is this detail that is so crucial to our understanding of the kinetics of the reaction. Consequently, what we need, in general, is to be able to quantify the rate of change of the dependent variable at a *particular* value of the independent variable rather than simply the average rate of change over some increment in the independent variable. This equates, in our chemical analogy, to being able to measure the instantaneous reaction rate at a given instant in time (and consequently for a given concentration of reactant or product), rather than the average rate of reaction over some extended period of time. However, before we can determine these instantaneous chemical rates, we must first establish some mathematical principles.

4.2 The Instantaneous Rate of Change

4.2.1 Differentiation from First Principles

If we now reconsider the general situation shown in Figure 4.1, we can determine the **instantaneous rate of change** by examining the limiting behaviour of the ratio, QR/PR, the change in y divided by the change in x, as Δx tends to zero:

$$\lim_{\Delta x \to 0}\left\{\frac{QR}{PR}\right\} = \lim_{\Delta x \to 0}\left\{\frac{\Delta y}{\Delta x}\right\} = \lim_{\Delta x \to 0}\left\{\frac{f(x_0 + \Delta x) - f(x_0)}{\Delta x}\right\} \quad (4.2)$$

The limiting value defined in equation (4.2) exists if:

- The function does not undergo any abrupt changes at x_0 (it is continuous at the point x_0).
- It is independent of the direction in which the point x_0 is approached.

If the limit in equation (4.2) exists, it is called the **derivative** of the function $y = f(x)$ at the point x_0. The value of the derivative varies with the choice of x_0, and we define it in general terms as:

$$\left(\frac{dy}{dx}\right)_{x=x_0} = \lim_{\Delta x \to 0}\left\{\frac{f(x_0 + \Delta x) - f(x_0)}{\Delta x}\right\} \quad (4.3)$$

where $\left(\frac{dy}{dx}\right)_{x=x_0}$ is the name given to the value of the derivative at the point x_0. The derivative of the function $y = f(x)$ at $x = x_0$ in Figure 4.1 corresponds geometrically to the slope of the tangent to the curve $y = f(x)$ at the point P (known as the **gradient**).

The basic formula (4.3) for the derivative is often given in the form:

$$\frac{dy}{dx} = \lim_{\Delta x \to 0}\left\{\frac{f(x + \Delta x) - f(x)}{\Delta x}\right\} \quad (4.4)$$

for an arbitrary value of x.

We should also note that:

- $\frac{dy}{dx}$ is the name of the **derivative function**, commonly also represented as $f'(x)$.
- The domain of the derivative function is not necessarily the same as that of $y = f(x)$ (see Table 4.1).

The requirement that, for the limit in equation (4.2) to exist, the function does not undergo any abrupt changes is sometimes overlooked, yet it is an important one. An example of a function falling into this category is the modulus function, $y = |x|$, defined by:

$$y = f(x) = |x| = \begin{cases} x & \text{if } x \geqslant 0 \\ -x & \text{if } x < 0 \end{cases}$$

This function is continuous for all values of x (Figure 4.2a), but there is no unique slope at the point $x = 0$ as the derivative is undefined at this point (Figure 4.2b).

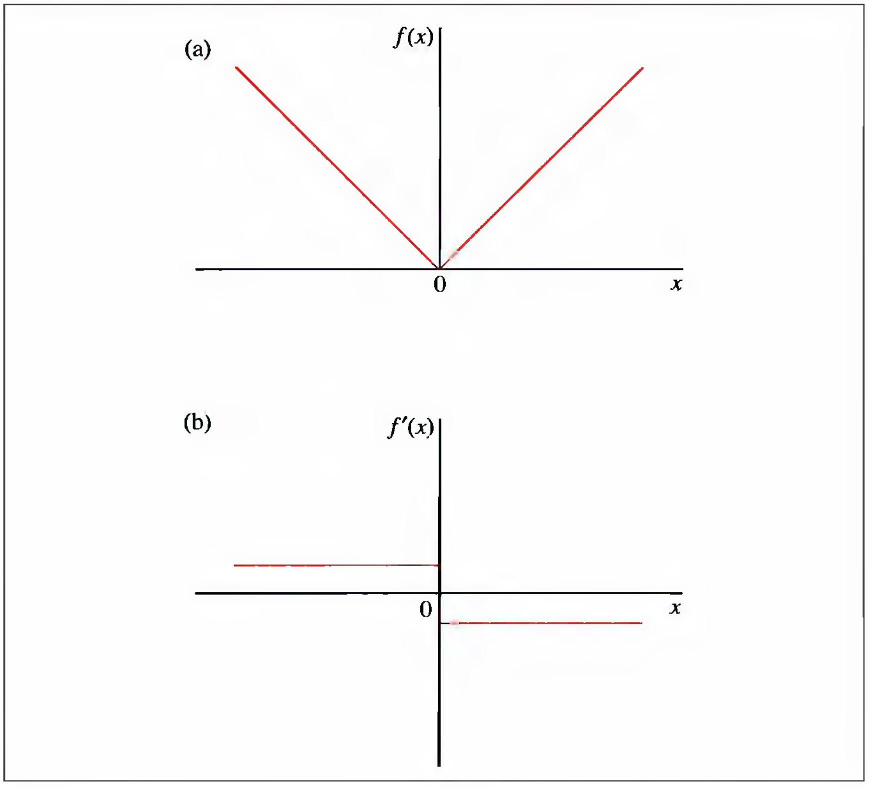

Figure 4.2 (a) The modulus function $y = f(x) = |x|$; (b) the derivative of the modulus function

Chemical examples showing this type of behaviour include processes associated with sudden changes in concentration, phase, crystal structure, temperature, *etc*. For example, Figure 2.9 shows how the equilibrium concentration of a chemical species changes suddenly when a temperature jump is applied at time t_0. Although there are no discontinuities in this function, its derivative is undefined at time t_0.

Worked Problem 4.1

Q Differentiate $y = f(x) = x^2$ using the definition of the derivative given in equation (4.4).

A $$\frac{dy}{dx} = \lim_{\Delta x \to 0}\left\{\frac{f(x+\Delta x) - f(x)}{\Delta x}\right\} = \lim_{\Delta x \to 0}\left\{\frac{(x+\Delta x)^2 - x^2}{\Delta x}\right\}$$

$$= \lim_{\Delta x \to 0}\left\{\frac{x^2 + 2x\Delta x + (\Delta x)^2 - x^2}{\Delta x}\right\} = \lim_{\Delta x \to 0}\left\{\frac{2x\Delta x + (\Delta x)^2}{\Delta x}\right\}$$

Since Δx tends to zero, but never takes the value zero, cancellation of Δx from all terms in the numerator and denominator yields:

$$\frac{dy}{dx} = \lim_{\Delta x \to 0}\{2x + \Delta x\} = 2x$$

Problem 4.1

Differentiate the function $y = f(x)$, where $f(x) = 3$, using the definition of the derivative given in equation (4.4). *Hint*: the function $y = f(x) = 3$ requires that $y = 3$ for all values of x; thus if $f(x) = 3$, then $f(x + \Delta x)$ must also equal 3.

Problem 4.2

Use equation (4.4) to find the derivative of the function $y = f(x)$, where (a) $f(x) = 3x^2$ and (b) $f(x) = 1/x^2$. *Hint*: in your answer to (b), you will need to remember how to subtract fractions, *i.e.* $\frac{1}{a} - \frac{1}{b} = \frac{b-a}{ab}$.

4.2.2 Differentiation by Rule

Some Standard Derivatives

The derivatives of all functions can be found using the limit method described in Section 4.2.1. Some of the more common functions, and their derivatives, are listed in Table 4.1. Unless otherwise indicated, the respective domains (Dom) are "all values of x":

Table 4.1 Derivatives of some common functions, and their respective domains

$f(x)$	$f'(x)$	Dom($f(x)$)	Dom($f'(x)$)	Notes
c	0	–	–	1
x^n	nx^{n-1} ($n \neq 0$)	$x \neq 0$ for $n<0$	$x \neq 0$ for $n<-1$	2
sin ax	a cos ax	–	–	3
cos ax	$-a$ sin ax	–	–	4
tan ax	$a\,\sec^2 ax$	$x \neq (2n+1)\pi/2$	$x \neq (2n+1)\pi/2$	5
sec ax	a sec ax tan ax	$x \neq (2n+1)\pi/2$	$x \neq (2n+1)\pi/2$	6
ln ax	a/x	$x>0$	$x \neq 0$	7
e^{ax}	$a.e^{ax}$	–	–	

[1]The constant function, c
[2]$n=0$ corresponds to the constant function
[3]$a \neq 0$; for a 1:1 function, Dom($f(x)$) = $[-\pi/2, \pi/2]$
[4]$a \neq 0$; for a 1:1 function, Dom($f(x)$) = $[0, \pi]$
[5,6,7]$a \neq 0$

However, as we have seen above, and in Table 4.1, we do meet functions for which the derivative $f'(x)$ does not exist at selected values of x. The functions $y = f(x) = \ln x$ at $x = 0$ and $y = f(x) = \tan x$ at $x = (2n + 1)\pi/2$, both listed in Table 4.1, fall into this category. Naturally, since the derivative does not exist in these cases at selective values of x, the domain of the derivatives of these functions will not be the same as the original functions. The restrictions on the respective domains are best seen in sample plots of these functions shown in Figure 4.3.

An Introduction to the Concept of the Operator

The notation $\frac{dy}{dx}$ (or sometimes dy/dx) for the derivative is just one of a number of different notations in widespread use, all of which are equivalent:

$$\frac{dy}{dx}, \quad dy/dx, \quad f'(x), \quad f^{(1)}(x), \quad \hat{D}f(x)$$

The more commonly used notations are $\frac{dy}{dx}$ and $f'(x)$, but expressing the derivative in the form $\hat{D}f(x)$ provides a useful reminder that the derivative function is obtained from the function $y = f(x)$ by the *operation* "differentiate with respect to x". Thus, we express this instruction in symbols as:

$$\hat{D}f(x) \equiv \frac{d}{dx}f(x) = \frac{d}{dx}y = \frac{dy}{dx} \tag{4.5}$$

It is worth emphasizing that the symbol $\frac{dy}{dx}$ does not mean dy divided by dx in this context, but represents the *limiting* value of the quotient $\Delta y/\Delta x$ as $\Delta x \to 0$.

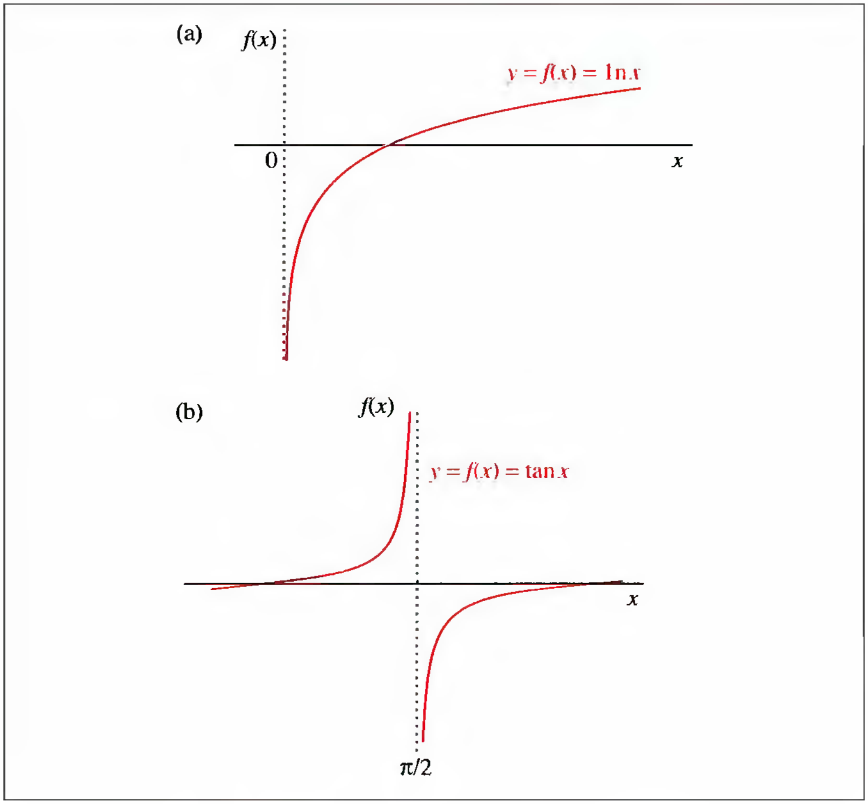

Figure 4.3 The functions (a) $y = f(x) = \ln x$ and (b) $y = f(x) = \tan x$ are both examples of functions for which the derivative does not exist at certain values in the independent variable (see Table 4.1)

In general, an **operator**, $\hat{A}$, is represented by a symbol with a caret ("hat") denoting an instruction to undertake an appropriate action on the object to its right (here $f(x)$). In equation (4.5), we consider $\frac{dy}{dx}$ to be the differentiation operator $\frac{d}{dx}$ acting on the function $f(x)$, which we have labelled y, to give a new function, say $g(x)$:

$$\hat{A}f(x) = g(x) \quad (4.6)$$

Worked Problem 4.2

Q For the function $f(x) = x^2$, find $\hat{A}(f(x))$ where $\hat{A} = d/dx$.

A For $f(x) = x^2$, $\frac{d}{dx}(f(x)) = 2x$.

Problem 4.3

For each of the following functions, $f(x)$, use the information in Table 4.1 to find $\hat{A}(f(x))$, where $\hat{A} = d/dx$: (a) $x^{3/4}$; (b) e^{-3x}; (c) $1/x$; (d) $a \cos ax$.

Problem 4.4

Use the information in Table 4.1 to demonstrate that, when the operator $\hat{A} = \frac{d}{dx} + 2$ acts on $f(x) = e^{-2x}$, the function is annihilated (*i.e.* the null function, $g(x) = 0$, results).

We will come to appreciate the full significance of the concept of the operator in Section 4.3.1, when we consider the *eigenvalue problem*.

4.2.3 Basic Rules for Differentiation

Although all functions can be differentiated from first principles, using equation (4.4), this can be a rather long-winded process in practice. In this chapter, we deal with the differentiation of more complicated functions with the aid of a set of rules, all of which may be derived from the defining relation (4.4). In many cases, however, we simply need to learn what the derivative of a particular function is, or how to go about differentiating a certain class of function. For example, we learn that the derivative of $y = f(x) = \sin x$ is $\cos x$, but that the derivative of $y = f(x) = \cos x$ is $-\sin x$. Similarly, we can differentiate any function of the type $y = f(x) = x^n$ by remembering the rule that we reduce the index of x by 1, and multiply the result by n; that is:

$$\frac{d}{dx}x^n = nx^{n-1} \qquad (n \neq 0) \tag{4.7}$$

For functions involving a combination of other elementary functions, we follow another set of rules: if u and v represent functions $f(x)$ and $g(x)$, respectively, then the rules for differentiating a sum, product or quotient can be expressed as:

$$\frac{d}{dx}(u + v) = \frac{du}{dx} + \frac{dv}{dx} \tag{4.8}$$

$$\frac{d}{dx}(uv) = v\frac{du}{dx} + u\frac{dv}{dx} \tag{4.9}$$

$$\frac{d}{dx}\left(\frac{u}{v}\right) = \frac{v\frac{du}{dx} - u\frac{dv}{dx}}{v^2} \tag{4.10}$$

Problem 4.5

Differentiate the following, using the appropriate rules: (a) $(x-1)(x^2+4)$; (b) $\frac{x}{(x+1)}$; (c) $\sin^2 x$; (d) $x \ln x$; (e) $e^x \sin x$.