2 Limits, Derivatives and Series

2.1 DEFINITION OF A LIMIT

Given a function $y = f(x)$ and a constant a: If there is a number, say γ, such that the value of $f(x)$ is as close to γ as desired, where x is different from a, then the limit of $f(x)$ as x approaches a is equal to γ. This formalism is then written as,

$$\lim_{x \to a} f(x) = \gamma. \tag{1}$$

A graphical interpretation of this concept is shown in Fig. 1.

If there is a value of ε such that $|f(x) - \gamma| < \varepsilon$, then x can be chosen anywhere at a value δ from the point $x = a$, with $0 < |x - a| < \delta$. Thus it is possible in the region near $x = a$ on the curve shown in Fig. 1, to limit the variation in $f(x)$ to as little as desired by simply narrowing the vertical band around $x = a$. Thus, Eq. (1) is graphically demonstrated. It should be emphasized that the existence of the limit given by Eq. (1) does not necessarily mean that $f(a)$ is defined.

As an example, consider the function

$$y(x) = \frac{\sin x}{x}. \tag{2}$$

The function $\sin x$ can be defined by an infinite series, as given in Eq. (1-35). Division by x yields the series

$$\frac{\sin x}{x} = 1 - \frac{x^2}{3!} + \frac{x^4}{5!} - \cdots. \tag{3}$$

It is evident from the right-hand side of Eq. (3) that this function becomes equal to 1 as x approaches zero, even though $y(0) = \frac{0}{0}$.* Thus, from a mathematical point of view it is not continuous, as it is not defined at $x = 0$. This function, which is of extreme importance in the applications of the Fourier transform (Chapter 11), is presented in Fig. 2.

*This result, $\frac{0}{0}$, is the most common indeterminate form (see Section 2.8).

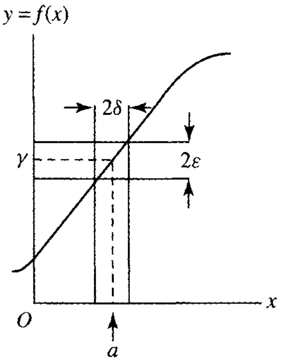

Fig. 1 The limit of a function.

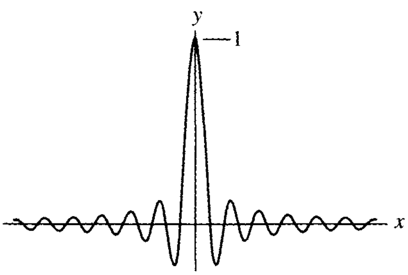

Fig. 2 The function $y(x) = \frac{sin\, x}{x}$.

It should be noted that computer programs written to calculate $y(x) = sin\, x/x$ will usually fail at the point $x = 0$. The computer will display a "division by zero" error message. The point $x = 0$ must be treated separately and the value of the limit ($y = 1$) inserted. However, "intelligent" programs such as *Mathematica** avoid this problem.

It is often convenient to consider the limiting process described above in the case of a function such as shown in Fig. 3. Then, it is apparent that the limiting value of $f(x)$ as $x \to a$ depends on the direction chosen. As x approaches a from the left, that is, from the region where $x < a$,

$$\lim_{x \to a_-} f(x) = \gamma_- . \tag{4}$$

**Mathematica*, Wolfram Research, Inc., Champaign, Ill., 1997.

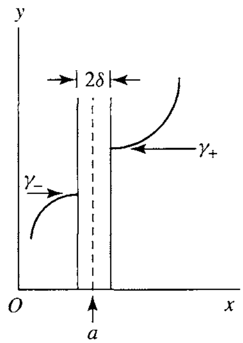

Fig. 3 The limits of the function $f(x)$ as x approaches a.

Similarly, from the right the limit is given by

$$\lim_{x \to a_+} f(x) = \gamma_+. \tag{5}$$

Clearly, in this example the two limits are not the same and this function cannot be evaluated at $x = a$. Another example is that shown in Fig. (1-3), where $P \to \infty$ as V approaches zero from the right (and $-\infty$, if the approach were made from the left).

2.2 CONTINUITY

The notion of continuity was introduced in Chapter 1. However, it can now be defined more specifically in terms of the appropriate limits.

A function $f(x)$ is said to be continuous at the point $x = a$ if the following three conditions are satisfied:

(i) The function is defined at $x = a$, namely, $f(a)$ exists,
(ii) The function approaches a limit as x approaches a (in either direction), *i.e.* $\lim_{x \to a} f(x)$ exists and
(iii) The limit is equal to the value of the function at the point in question, *i.e.* $\lim_{x \to a} f(x) = f(a)$.

See problem 3 for some applications.

The rules for combining limits are, for the most part, obvious:

(i) The limit of a sum is equal to the sum of the limits of the terms; thus, $\lim_{x \to a}[f(x) + g(x)] = \lim_{x \to a} f(x) + \lim_{x \to a} g(x)$.

(ii) The limit of a product is equal to the product of the limits of the factors; then $lim_{x\to a}[f(x)\cdot g(x)] = lim_{x\to a} f(x)\cdot lim_{x\to a} g(x)$ and hence $lim_{x\to a}[f(cx)] = c\, lim_{x\to a} f(x)$, where c is an arbitrary constant.

(iii) The limit of the quotient of two functions is equal to the quotient of the limits of the numerator and denominator, if the limit of the denominator is different from zero, *viz.*

$$\lim_{x\to a}\frac{f(x)}{g(x)} = \frac{\lim_{x\to a} f(x)}{\lim_{x\to a} g(x)}, \quad \text{if } \lim_{x\to a} g(x) \neq 0.$$

Rule (iii) is particularly important in the tests for series convergence that will be described in Section 2.11.

An additional question arises in the application of rule (iii) when both the numerator and the denominator approach zero. This rule does not then apply; the ratio of the limits becomes in this case $\frac{0}{0}$, which is undefined. However, the limit of the ratio may exist, as found often in the applications considered in the following chapters. In fact, an example has already been presented [see Eq. (2)].

2.3 THE DERIVATIVE

Given a continuous function $y = f(x)$, for a given value of x there is a corresponding value of y. Now, consider another value of x which differs from the first one by an amount Δx, which is referred to as the increment of x. For this value of x, y will have a different value which differs from the first one by a quantity Δy. Thus,

$$y + \Delta y = f(x + \Delta x) \tag{6}$$

or

$$\Delta y = f(x + \Delta x) - f(x) \tag{7}$$

and

$$\frac{\Delta y}{\Delta x} = \frac{f(x + \Delta x) - f(x)}{\Delta x}. \tag{8}$$

In the limit as both the numerator and the denominator of Eq. (8) approach zero, the finite differences Δy and Δx become the (infinitesimal) differentials $\mathrm{d}y$ and $\mathrm{d}x$. Thus, Eq. (8) takes the form

$$\frac{\mathrm{d}y}{\mathrm{d}x} = \lim_{\Delta x\to 0}\frac{\Delta y}{\Delta x} = \lim_{\Delta x\to 0}\frac{f(x + \Delta x) - f(x)}{\Delta x}, \tag{9}$$

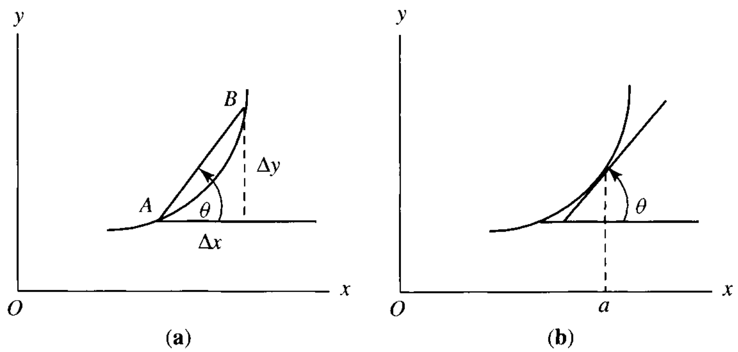

Fig. 4 The derivative: (**a**) Definitions of Δx and Δy; (**b**) $\tan\theta = \dfrac{dy}{dx}$.

which is called the derivative of y with respect to x. The notation $y' \equiv dy/dx$ is often used if there is no ambiguity regarding the independent variable x. The derivative exists for most continuous functions. As shown in elementary calculus, the requirements for the existence of the derivative in some range of values of the independent variable, are that it be continuous, single-valued and differentiable, that is, that y be an analytic function of x.

A graphical interpretation of the derivative is introduced here, as it is extremely important in practical applications. The quantities Δx and Δy are identified in Fig. 4a. It should be obvious that the ratio, as given by Eq. (8) represents the tangent of the angle θ and that in the limit (Fig. 4b), the slope of the line segment $\overline{AB}$ (the secant) becomes equal to the derivative given by Eq. (8).

It was already assumed in Chapter 1 that readers are familiar with the methods for determining the derivatives of algebraic functions. The general rules, as proven in all basic calculus courses, can be summarized as follows.

(i) Derivative of a constant:

$$\frac{da}{dx} = 0, \tag{10}$$

where a is a constant.

(ii) Derivative of a sum:

$$\frac{d}{dx}(u + v) = \frac{du}{dx} + \frac{dv}{dx}, \tag{11}$$

where u and v are functions of x.

(iii) Derivative of a product:

$$\frac{d}{dx}(uv) = u\frac{dv}{dx} + v\frac{du}{dx}. \tag{12}$$

(iv) Derivative of a quotient:

$$\frac{d}{dx}\left(\frac{u}{v}\right) = \frac{v\frac{du}{dx} - u\frac{dv}{dx}}{v^2}. \tag{13}$$

(v) Derivative of a function of a function:
Given the function $y[u(x)]$,

$$\frac{dy}{dx} = \frac{dy}{du} \cdot \frac{du}{dx}. \tag{14}$$

Equation (14) leads immediately to the relations

$$\frac{dy}{dx} = \frac{\frac{dy}{du}}{\frac{dx}{du}} \text{ if } \frac{dx}{du} \neq 0$$

and

$$\frac{dy}{dx} = \frac{1}{\frac{dx}{dy}} \text{ if } \frac{dx}{dy} \neq 0.$$

(vi) The power formula:

$$\frac{d}{dx}u^n = nu^{n-1}\frac{du}{dx} \tag{15}$$

for the function $u(x)$ raised to any power.

The derivative of the logarithm was already discussed in Chapter 1, while the derivatives of the various trigonometric functions can be developed from their definitions [see, for example, Eqs. (1-36), (1-37), (1-44) and (1-45)]. A number of expressions for the derivatives can be derived from the problems at the end of this chapter.

2.4 HIGHER DERIVATIVES

If y is a function of x, the derivative of $y(x)$ is also, in general, a function of x. It can then be differentiated to yield the second derivative of y with respect to x, namely,

$$y'' \equiv \frac{d^2y}{dx^2} = \frac{d}{dx}\frac{dy}{dx}. \tag{16}$$

It should be noted here that the operation of taking the derivative, that is, the result of the operator d/dx operating on a function of x, followed by the same operation, yields the second derivative. Thus, the successive application of two operators is referred to as their product. This question is addressed more specifically in Chapter 7.

Clearly, y'' in Eq. (16) represents the rate of change of the slope of the function $y(x)$. The second derivative can be expressed in terms of derivatives with respect to y, *viz.*,

$$\frac{dy'}{dx} = \frac{\dfrac{dy'}{dy}}{\dfrac{dx}{dy}}, \tag{17}$$

which leads to

$$y'' \equiv \frac{d^2y}{dx^2} = -\frac{\dfrac{d^2x}{dy^2}}{\left(\dfrac{dx}{dy}\right)^3}, \tag{18}$$

a relation which is sometimes useful.

2.5 IMPLICIT AND PARAMETRIC RELATIONS

Often two variables x and y are related implicitly in the form $f(x, y) = 0$. Although it is sometimes feasible to solve for y as a function of x, such is not always the case. However, if rule (vi) above [Eq. (15)] is applied with care, the derivatives can be evaluated. As an example, consider the equation for a circle of radius r,

$$x^2 + y^2 = r^2. \tag{19}$$

Rather than to solve for y, it is more convenient to apply rule (vi) directly; then $2x + 2y(dy/dx) = 0$ and $y' = dy/dx = -x/y$. The second derivative is then obtained with the use of rule (iv):

$$\frac{d^2y}{dx^2} = \frac{xy' - y}{y^2}.$$

Sometimes the two variables are expressed in terms of a third variable, or parameter. Then, $x = u(t)$ and $y = v(t)$ and, in principle, the parameter t can be eliminated to obtain a relation between x and y. Here again, this operation is not always easy, or even, possible. An example is provided by the pair of equations $x = t^2 + 2t - 4$ and $y = t^2 - t + 2$. The two derivatives dx/dt and dy/dt are easily obtained and, with the aid of rule (v), their ratio becomes

$$\frac{dy}{dx} = \frac{3t^2 - 1}{3t^2 + 2}.$$

The second derivative is then given by

$$\frac{d^2y}{dx^2} = \frac{18t}{(3t^2 + 2)^3},$$

where the relations below Eq. (14) have been employed. This result is left as an exercise for the reader (problem 7).

2.6 THE EXTREMA OF A FUNCTION AND ITS CRITICAL POINTS

As shown in Fig. 4b, the derivative of a function evaluated at a given point is equal to the slope of the curve at that point. Given two points x_1 and x_2 in the neighborhood of a such that $x_1 < a$ and $x_2 > a$, it is apparent that if $f(x_1) < f(a) < f(x_2)$, the slope is positive. Similarly, if $f(x_1) > f(a) > f(x_2)$ in the same region, the slope is negative. On the other hand, if $f(x_1) < f(a) > f(x_2)$ the function has a maximum value in the neighborhood of a. It is of course minimal in that region if $f(x_1) > f(a) < f(x_2)$. At either a maximum or a minimum the derivative of the function is zero. Thus, the slope is equal to zero at these points, which are the *extrema*, as shown by points a and c in Fig. 5. A function may have additional maxima or minima in other regions. In Fig. 5 there are maxima at $x = a$ and $x = b$. As $f(a) > f(b)$, the point a is called the absolute or principal maximum and that at b is a submaximum.

It should be obvious from Fig. 5 that the curve is concave upward at a minimum (c) and downward at a maximum, such as a and b. As the second derivative of the function is the rate of change of the slope, the sign of the second derivative provides a method of distinguishing a minimum from a maximum. In the former case the second derivative is positive, while in the latter it is negative. The value of the second derivative at an extreme point is referred to as the curvature of the function at that point.

A case that has not yet been considered in this section is shown in Fig. 5 at the point $x = d$. At this point the slope of the first derivative is equal to zero, that is

$$\left.\frac{d^2f}{dx^2}\right|_{x=d} = 0.$$

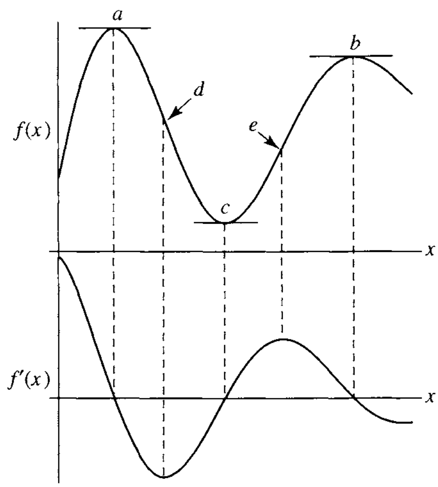

Fig. 5 A function $f(x)$ and its derivative, $f'(x)$.

Hence the point $x = d$ is neither a maximum nor a minimum of the function $f(x)$. Here, $f(x_1) > f(d) > f(x_2)$ and, as $x_1 < d < x_2$, the slope is not equal to zero. The point $x = d$ is known as an inflection point, a point at which the second derivative or curvature is zero. The point $x = e$ is also an inflection point, as $f'' = 0$. The ensemble of extrema and inflection points of a function are known as its critical points.

An example of a function which exhibits an inflection point is provided by the well-known equation of Van der Waals,* which for one mole of a gas takes the form,

$$\left(P + \frac{a}{V^2}\right)(V - b) = RT, \tag{20}$$

where a and b are constants. The derivative can be obtained in the form

$$\left(\frac{\partial P}{\partial V}\right)_T = \frac{-RT}{(V-b)^2} + \frac{2a}{V^3}, \tag{21}$$

where the subscript T indicates that the temperature has been held constant.† Note that the slope is equal to zero at infinite molar volume and becomes infinite at $V = b$. However, there is an intermediate point of interest along the curve $T = T_c$. At this, the so-called critical point, the curve exhibits an

*Johannes Diderik Van der Waals, Dutch physicist (1887–1923).

†The derivative in Eq. (21) is an example of a partial derivative, a subject that will be treated at the end of this chapter.

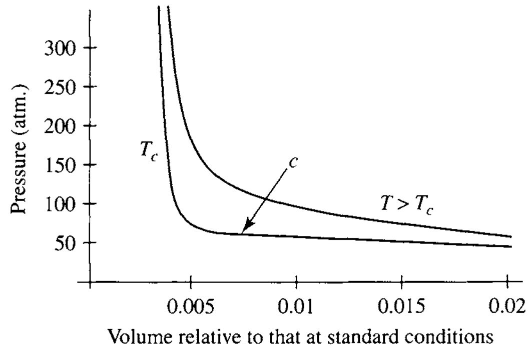

Fig. 6 Isotherms of a Van der Waals fluid; the critical point is shown at c (1 atm. = 101 kPa).

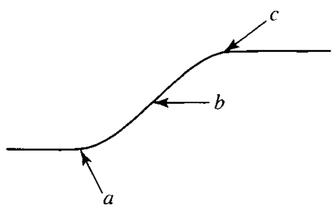

Fig. 7 Profile of a road.

inflection point, as shown in Fig. 6. At this point the derivative of Eq. (21) is equal to zero and the corresponding molar volume is given by $V_c = 3b$. The development of this result is left as an exercise (see problem 5).

It should be noted that the isotherm which passes through the critical point (Fig. 6) is a "smooth curve" in the sense that both the function $P(V)$ and its first derivative are continuous. However, the second derivative at the critical point is not.

Another, more everyday example of this behavior occurs in road construction. An automobile begins its ascent of a grade at point a in Fig. 7. The pavement is both unbroken (the function is continuous) and smooth (its derivative is continuous). However, at point a, as well as at points b and c, the second derivative, which represents the rate of change in the grade, is discontinuous.

2.7 THE DIFFERENTIAL

When the change in a variable, say Δx, approaches zero it is called an infinitesimal. The branch of mathematics known as analysis, or the calculus, is based on this principle, as both Δx and Δy approach zero in the limit [see Eq. (8)]. For practical purposes the derivative $\mathrm{d}y/\mathrm{d}x$ can be decomposed into differentials in the form $\mathrm{d}y = (\mathrm{d}y/\mathrm{d}x)\mathrm{d}x$. While this operation deserves some justification from a purely mathematical point of view, it is correct for the purposes of this book.

In this context Eq. (12) can be rewritten in the form of differentials as

$$\mathrm{d}(uv) = u\,\mathrm{d}v + v\,\mathrm{d}u. \tag{22}$$

In other words the differential of a product of two functions is equal to the first function times the differential of the second, plus the second times the differential of the first. Numerous examples of this principle will be encountered in the exercises at the end of this chapter, as well as in following chapters. The other rules presented above can easily be modified accordingly.

A geometrical interpretation of the differential is represented in Fig. 8. It is apparent that in general $\mathrm{d}y < \Delta y$ or $\mathrm{d}y > \Delta y$, as the curve is concave upward or downward, respectively.

It is often useful to evaluate the differential along a curve s such as shown in Fig. 9. Let Δs be the length of the curve $y = f(x)$ measured between points a and b and assume that s increases as x increases. Thus, the derivative can be expressed as

$$\frac{\mathrm{d}s}{\mathrm{d}x} = \lim_{\Delta x \to 0} \frac{\Delta\sigma}{\Delta x} = \sqrt{1 + \left(\frac{\mathrm{d}y}{\mathrm{d}x}\right)^2} \tag{23}$$

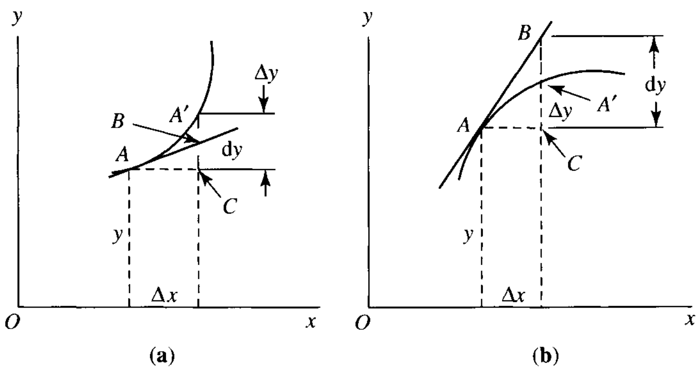

Fig. 8 Geometrical interpretation of the differential.

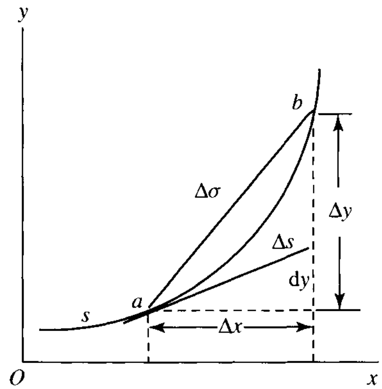

Fig. 9 Geometrical illustration of the infinitesimal of arc, d*s*.

and, as Δs approaches $\Delta\sigma$ in the limit,

$$\overline{\mathrm{d}s}^2 = \overline{\mathrm{d}x}^2 + \overline{\mathrm{d}y}^2. \tag{24}$$

Then the differential ds becomes the hypotenuse of the triangle shown in Fig. 9. The same result is obtained if s decreases as x increases.

2.8 THE MEAN-VALUE THEOREM AND L'HOSPITAL'S RULE*

An important theorem, often attributed to Lagrange,† can be written in the form

$$f'(x_1) = \frac{f(b) - f(a)}{b - a}. \tag{25}$$

Here $f'(x_1)$ is the derivative $\mathrm{d}y/\mathrm{d}x$ evaluated at a point x_1 which is intermediate with respect to points a and b. From Fig. 10 it should be evident that there is always some point $x = x_1$ where the slope of the curve is equal to the right-hand side of Eq. (25). This theorem will be employed in Chapter 13 to evaluate the error in linear interpolation.

If two functions $f(x)$ and $g(x)$ both vanish at a point a, the ratio $f(a)/g(a)$ is undefined. It is the so-called indeterminate form $\frac{0}{0}$ mentioned earlier

*Guillaume de L'Hospital, French mathematician (1661–1704).

†Louis de Lagrange, French mathematician (1736–1813).

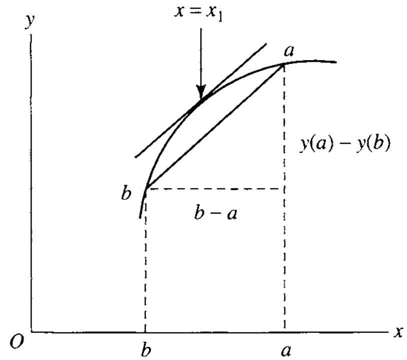

Fig. 10 The slope of a curve at $x = x_1$.

(Sections 2.1 and 2.2). However, the limit of this ratio may exist. In fact this principle is the very basis of the differential calculus, as indicated by Eq. (9).

Consider now Eq. (25), with b replaced by x, *viz.*

$$f(x) = (x - a)f'(x_1) + f(a). \tag{26}$$

Similarly, for another function $g(x)$,

$$g(x) = (x - a)g'(x_2) + g(a); \tag{27}$$

and, as the case of interest is $f(a) = g(a) = 0$, Eqs. (26) and (27) yield

$$\frac{f(x)}{g(x)} = \frac{f'(x_1)}{g'(x_2)}. \tag{28}$$

Because both x_1 and x_2 lie between x and a, they both must approach a as x does. Thus,

$$\lim_{x \to a} \frac{f(x)}{g(x)} = \lim_{x \to a} \frac{f'(x)}{g'(x)}, \tag{29}$$

which is known as L'Hospital's rule. A trivial example of its application is provided by the function $\sin x/x$. In this case the ratio of the first derivatives evaluated at the origin is equal to unity, as shown earlier.

An example which may be familiar to chemists, as it arises in extraction and fractional distillation, is the function

$$y = \frac{x^{n+1} - x}{x^{n+1} - 1}, \tag{30}$$

where n is an integer. This function is undefined at $x = 1$. However, with the application of Eq. (29), the limit is given by

$$\lim_{x\to 1} \frac{x^{n+1} - x}{x^{n+1} - 1} = \lim_{x\to 1} \frac{(n+1)x^n - 1}{(n+1)x^n} = \frac{n}{n+1} \tag{31}$$

for all finite values of n.

L'Hospital's rule has been applied above to cases in which the indeterminate form is $\frac{0}{0}$. However, it is equally valid for the form $\frac{\infty}{\infty}$.

2.9 TAYLOR'S SERIES*

Power series have already been introduced to represent a function. For example, Eq. (1-35) expresses the function $y = \sin x$ as a sum of an infinite number of terms. Clearly, for $x < 1$, terms in the series become successively smaller and the series is said to be convergent, as discussed below. The numerical evaluation of the function is carried out by simply adding terms until the value is obtained with the desired precision. All computer operations used to evaluate the various irrational functions are based on this principle.

Now assume that a given function can be differentiated indefinitely at a given point a and that its expansion in a power series is of the form

$$f(x) = c_0 + c_1(x-a) + c_2(x-a)^2 + c_3(x-a)^3 + \cdots . \tag{32}$$

If this series converges in the region around the point a, it can be used to calculate the function $f(x)$ to a precision determined by the number of terms retained. Assuming that the series exists, the coefficients can be determined. Certainly, $c_0 = f(a)$ and, by successive, term-by-term differentiation the subsequent coefficients are evaluated. Thus, as

$$f'(x) = c_1 + 2c_2(x-a) + 3c_3(x-a)^2 + 4c_4(x-a)^3 + \cdots , \tag{33}$$
$$f'(a) = c_1,$$

and

$$f''(a) = 2 \cdot 1c_2$$
$$f'''(a) = 3 \cdot 2 \cdot 1c_3$$
$$\vdots$$
$$f^{(n)}(a) = n!c_n.$$

*Brook Taylor, British mathematician (1685–1731).

The general form of Taylor's series is then

$$f(x) = f(a) + f'(a)(x-a) + \frac{1}{2!}f''(a)(x-a)^2 + \frac{1}{3!}f'''(a)(x-a)^3 + \cdots + \frac{1}{n!}f^{(n)}(a)(x-a)^n + \cdots. \tag{34}$$

Thus, it has been shown that if a series as presented in Eq. (32) exists, it is given by Eq. (34). However, the function and its successive derivatives must be defined at $x = a$. Furthermore, the function must be analytic, the series must be convergent in this region and the value obtained must be equal to $f(x)$. These questions deserve further consideration for a given problem.

An example of the development of a Taylor's series is provided by the expansion of the function $ln\, x$ around the point $x = 1$. The necessary derivatives become

$$\begin{aligned}
f'(x) &= \frac{1}{x} & f'(1) &= 1\\
f''(x) &= -\frac{1}{x^2} & f''(1) &= -1\\
f'''(x) &= \frac{2}{x^3} & f'''(1) &= 2\\
f^{(iv)}(x) &= -\frac{2\cdot 3}{x^4} & f^{(iv)}(1) &= -2\cdot 3\\
&\vdots & &\vdots\\
f^{(n)}(x) &= (-1)^{n-1}\frac{(n-1)!}{x^n} & f^{(n)}(1) &= (-1)^{n-1}(n-1)!\\
&\vdots & &\vdots
\end{aligned}$$

and the series is then

$$ln\, x = (x-1) - \frac{(x-1)^2}{2} + \frac{(x-1)^3}{3} - \cdots + (-1)^{n-1}\frac{(n-1)^n}{n} + \cdots . \tag{35}$$

It can be shown that this series converges for $0 < x \leq 2$ (see Section 2.11).

An important special case of Taylor's series occurs when $a = 0$. Then, Eq. (34) takes the form

$$f(x) = f(0) + f'(0)x + \frac{1}{2!}f''(0)x^2 + \frac{1}{3!}f'''(0)x^3 + \cdots + \frac{1}{n!}f^{(n)}(0)x^n + \cdots, \tag{36}$$

which is known as Maclaurin's series.* An application was introduced in Chapter 1, where one definition of the function *sin x* was expressed as an infinite series [see Eq. (1-35) and problem 9].

2.10 BINOMIAL EXPANSION

Consider the development of the function $(x+1)^\alpha$ in a Maclaurin series,

$$f(x) = 1 + \alpha x + \frac{\alpha(\alpha-1)}{2!}x^2 + \cdots + \frac{\alpha(\alpha-1)\cdots(\alpha-n+1)}{n!}x^n + \cdots. \tag{37}$$

The coefficients are known in the form

$$\binom{\alpha}{n} \equiv \frac{\alpha(\alpha-1)\cdots(\alpha-n+1)}{n!} \tag{38}$$

as the binomial coefficients. In the special case in which $\alpha = n$, a positive integer,

$$\binom{n}{n} = 1$$

and

$$\binom{n}{n+1} = \binom{n}{n+2} = \cdots = 0.$$

The infinite series given by Eq. (37) then reduces to the polynomial

$$(x+1)^n = 1 + \binom{n}{1}x + \binom{n}{2}x^2 + \cdots + \binom{n}{n}x^n, \tag{39}$$

which is Newton's binomial formula.†

The binomial expansion, Eq. (37), is particularly useful in numerical applications. For example, if $\alpha = \frac{1}{2}$,

$$f(x) = (x+1)^{1/2} = 1 + \frac{x}{2} - \frac{x^2}{8} + \frac{x^3}{16} - \cdots. \tag{40}$$

*Colin Maclaurin, Scottish mathematician (1698–1746).

†Sir Isaac Newton, English physicist and mathematician (1642–1727).

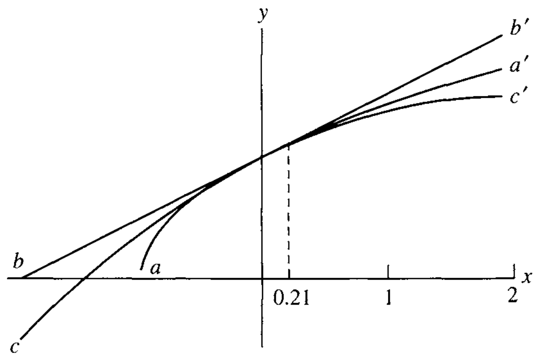

Fig. 11 (a) The function $y = (x + 1)^{1/2}$; (b) Linear approximation; (c) Quadratic approximation.

This function is shown in Fig. 11, where it is compared with the two- and three-term approximations derived from Eq. (40). At values of x near zero these approximations become increasingly accurate. If, for example, $x = 0.2100$, $y = (1 + 0.2100)^{1/2} = 1.1000$, while the two-term approximation yields $y = 1 + 0.2100/2 = 1.1050$. This development is often employed in computer programs. Clearly, for a given value of x the number of terms used is determined by the precision required in the numerical result.

2.11 TESTS OF SERIES CONVERGENCE

The most useful test for the convergence of a series is called Cauchy's ratio test.* It can be summarized as follows for a series defined by Eq. (32).

(i) If $lim_{n\to\infty} |c_{n+1}/c_n| < 1$ the series converges absolutely,† and thus converges.

(ii) If $lim_{n\to\infty} |c_{n+1}/c_n| > 1$, or if $|c_{n+1}/c_n|$ increases indefinitely, the series diverges.

(iii) If $lim_{n\to\infty} |c_{n+1}/c_n| = 1$ or if the quantity $|c_{n+1}/c_n|$ does not approach a limit and does not increase indefinitely, the test fails.

*Augustin Cauchy, French mathematician (1789–1857).

†A series is said to be absolutely convergent if the series formed by replacing all of its terms by their absolute values is convergent.

As an example, consider the series

$$y = e^x = 1 + x + \frac{1}{2!}x^2 + \frac{1}{3!}x^3 + \cdots = \sum_{n=0}^{\infty} \frac{x^n}{n!}, \tag{41}$$

which was introduced in Chapter 1 as a definition of the exponential function. Application of the ratio test yields

$$\lim_{n\to\infty} \frac{x^{n+1}/(n+1)!}{x^n/n!} = \lim_{n\to\infty} \frac{x}{n} = 0 \; ; \tag{42}$$

thus the series converges for all finite values of x.

Another test can be applied in the case of an alternating series, that is, one in which the terms are alternately positive and negative. It can be shown that if, after a certain number of terms, further terms do not increase in value and that the limit of the n^{th} term is zero, the series is convergent.

As an example, consider the series

$$\sin x = x - \frac{x^3}{3!} + \frac{x^5}{5!} - \frac{x^7}{7!} + \cdots = \sum_{n=0}^{\infty} \frac{(-1)^n x^{2n}}{(2n)!}, \tag{43}$$

which was introduced in Section 1.7 [see Eq. (1-35)]. This series is alternating, with successive terms decreasing in absolute value. Furthermore, as

$$\lim_{n\to\infty} \frac{x^{2n}}{(2n)!} = 0, \tag{44}$$

the power series which defines the sine function is convergent for all finite values of x.

Two other important considerations are involved in the use of infinite series. Convergence may be assured only within a given range of the independent variable, or even only at a single point. Thus, the "region of convergence" can be identified for a given series. The reader is referred to textbooks on advanced calculus for the analysis of this problem.

A second question arises in practical applications, because at different points within the region of convergence, the rate of convergence may be quite different. In other words the number of terms that must be retained to yield a certain level of accuracy depends on the value of the independent variable. In this case the series is not uniformly convergent.

2.12 FUNCTIONS OF SEVERAL VARIABLES

Thus far in this chapter, functions of only a single variable have been considered. However, a function may depend on several independent variables. For example, $z = f(x,y)$, where x and y are independent variables. If one of these variables, say y, is held constant, the function depends only on x. Then, the derivative can be found by application of the methods developed in this chapter. In this case the derivative is called the partial derivative of z with respect to x, which is represented by $\partial z/\partial x$ or $\partial f/\partial x$. The partial derivative with respect to y is analogous. The same principle can be applied to implicit functions of several independent variables by the method developed in Section 2.5. Clearly, the notion of partial derivatives can be extended to functions of any number of independent variables. However, it must be remembered that when differentiating with respect to a given independent variable, all others are held constant.

Higher derivatives are obtained by obvious extension of this principle. Thus,

$$\frac{\partial}{\partial x}\left(\frac{\partial z}{\partial x}\right) = \frac{\partial^2 z}{\partial x^2},$$

as in Section 2.4 [See Eq. (16)]. It should be noted, however, that the order of differentiation is unimportant if the function $z(x,y)$ is continuous. So that

$$\frac{\partial^2 z}{\partial x \partial y} = \frac{\partial^2 z}{\partial y \partial x},$$

a relation that is important, as shown in the following chapter.

It is now of interest to define the total differential by the relation

$$dz = \left(\frac{\partial z}{\partial x}\right) dx + \left(\frac{\partial z}{\partial y}\right) dy. \tag{45}$$

This expression is a simple generalization of the argument developed in Section 2.7. It, and its extension to functions of any number of variables, is referred to as the "chain rule". In many applications it is customary to add one or more subscripts to the partial derivatives to specify the one or more variables that were held constant. As an example, Eq. (45) becomes

$$dz = \left(\frac{\partial z}{\partial x}\right)_y dx + \left(\frac{\partial z}{\partial y}\right)_x dy. \tag{46}$$

This notation was suggested in Eq. (21) and is usually employed in thermodynamic applications.

2.13 EXACT DIFFERENTIALS

Equation (45) can be written in the general form

$$\delta z = M(x,y)\,\mathrm{d}x + N(x,y)\,\mathrm{d}y. \tag{47}$$

However, in the special case in which $M(x,y) = \partial z/\partial x$ and $N(x,y) = \partial z/\partial y$ the differential can be identified with that given by Eq. (45). As the order of differentiation is unimportant, the relation

$$\frac{\partial M}{\partial y} = \frac{\partial^2 z}{\partial y \partial x} = \frac{\partial^2 z}{\partial x \partial y} = \frac{\partial N}{\partial x} \tag{48}$$

is easily obtained. The total differential, which is then said to be exact, is written dz to distinguish it from the inexact differential denoted δz. The condition for exactness, as given by Eq. (48), namely,

$$\frac{\partial M}{\partial y} = \frac{\partial N}{\partial x} \tag{49}$$

is attributed to either Cauchy or Euler, depending on the author.

In thermodynamics the eight quantities P, V, T, E, S, H, F and G are the state functions, pressure, volume, temperature, energy, entropy, enthalpy, Helmholtz* free energy and Gibbs† free energy, respectively. By definition, all of the corresponding differentials are exact (see Section 3.5). The thermodynamics of systems of constant composition can be developed with the use of any of the following sets of three state functions: E,S,V; H,S,P; F,T,V; G,T,P. Thus, for example, with $E = f(S,V)$

$$\mathrm{d}E = \left(\frac{\partial E}{\partial S}\right)_V \mathrm{d}S + \left(\frac{\partial E}{\partial V}\right)_S \mathrm{d}V. \tag{50}$$

However, the first law of thermodynamics expresses the differential dE as

$$\mathrm{d}E = \delta q + \delta w, \tag{51}$$

where the additional quantities q, the heat, and w the work have been introduced.‡ Note that these two important thermodynamic quantities are not state

*Hermann von Helmholtz, German physicist and physiologist (1821–1894).

†J. Willard Gibbs, American chemical physicist (1839–1903).

‡The convention adopted here is that δw is negative if work is done by the system. However, in some textbooks the first law of thermodynamics is written in the form d$E = \delta q - \delta w$, in which case the work done by the system is positive.

functions; thus, their differentials are not exact. However, for a gas under reversible conditions $\delta w = -P\,\mathrm{d}V$, while from the definition of the entropy as given in Section 3.5, $\delta q = T\,\mathrm{d}S$. The resulting expression,

$$\mathrm{d}E = T\,\mathrm{d}S - P\,\mathrm{d}V \tag{52}$$

can be compared to Eq. (50) to yield the relations

$$\left(\frac{\partial E}{\partial S}\right)_V = T \text{ and } \left(\frac{\partial E}{\partial V}\right)_S = -P.$$

The application of the condition given by Eq. (49) leads to one of the four Maxwell relations,* *viz.*

$$\left(\frac{\partial T}{\partial V}\right)_S = -\left(\frac{\partial P}{\partial S}\right)_V. \tag{53}$$

The other three can be derived similarly (see problem 10 and Section 7.6).

PROBLEMS

1. Find the first derivatives of the following functions:

$y = \dfrac{x-1}{\sqrt{x^2+1}}$; Ans. $y' = \dfrac{x+1}{(x^2+1)^{3/2}}$

$y = \dfrac{1}{x^2} + \sqrt[3]{(x^3 + cos^3 x)^2}$ Ans. $y' = -\dfrac{2}{x^3} + \dfrac{2(2x - 3\, sin\, x\, cos^2 x)}{3\sqrt[3]{x^2 + cos^3 x}}$

$y = \dfrac{x^2+1}{4x+3}$ Ans. $y' = \dfrac{2(2x-1)(x+2)}{(4x+3)^2}$

$y = tan(x\, sin\, x)$ Ans. $y' = (x\, cos\, x + sin\, x)\, sec^2(x\, sin\, x)$

$y = sec^2 x - tan^2 x$ Ans. $y' = 0$

2. Given the curve $y = cos\, x$, find the points where the tangent is parallel to the x axis. Ans. $x = k\pi, k = 0, \pm1, \pm2, \cdots$

3. Evaluate the following limits:

$\lim\limits_{\alpha\to 0} \dfrac{sin\, k\alpha}{\alpha}$ Ans. k

*James Clark Maxwell, British physicist (1831–1879).

$\lim_{x \to 2} (x^3 - 3x)$ Ans. 2

$\lim_{x \to 2} \frac{x^3 - x^2 + 2x - 8}{x - 2}$ Ans. 10

$\lim_{x \to 0} \frac{x + \tan x}{\sin 3x}$ Ans. $\frac{2}{3}$

$\lim_{x \to 0} \frac{\sin x - x}{x^3}$ Ans. $-\frac{1}{6}$

4. Verify Eq. (21) and calculate the second partial derivative.

Ans. $\left(\frac{\partial^2 P}{\partial V^2}\right)_T = \frac{2RT}{(V-b)^3} - \frac{6a}{V^4}$

5. Show that for a Van der Waals' fluid at the critical point

$$T_c = \frac{a}{27Rb}, \ V_c = 3b \text{ and } P_c = \frac{a}{27b^2}$$

6. Given the relation

$$(a-b)kt = \ln \frac{b(a-x)}{a(b-x)},$$

where $a \neq b$ are constants, find the expression for dx/dt.

Ans. $\frac{dx}{dt} = \frac{abk(a-b)^2 e^{k(a-b)t}}{(ae^{k(a-b)t} - b)^2}$

7. Given $x = t^2 + 2t - 4$ and $y = t^2 - t + 2$, evaluate d^2y/dx^2.

Ans. *cf.* Section 2.5.

8. If $y = A \cos kx + B \sin kx$, where A, B and k are constants, find the expression for d^2y/dx^2.

Ans. $\frac{d^2y}{dx^2} = -k^2 y$

9. Verify the series for $\cos \varphi$ and $\sin \varphi$ given by Eqs. (1-34) and (1-35), respectively.

10. Verify Eq. (53) and derive the other three Maxwell relations, namely,

$$\left(\frac{\partial S}{\partial V}\right)_T = \left(\frac{\partial P}{\partial T}\right)_V, \quad \left(\frac{\partial T}{\partial P}\right)_S = \left(\frac{\partial V}{\partial S}\right)_P \quad \text{and} \quad \left(\frac{\partial S}{\partial P}\right)_T = -\left(\frac{\partial V}{\partial T}\right)_P.$$

11. Find the first partial derivatives of the function $z = 4x^2y - y^2 + 3x - 1$.

Ans. $\frac{\partial z}{\partial x} = 8xy + 3, \ \frac{\partial z}{\partial y} = 4x^2 - 2y$

12. Given $z^2 + 2zx = x^2 - y^2$, find the first partial derivatives z.

Ans. $\dfrac{\partial z}{\partial x} = \dfrac{x - z}{x + z}, \dfrac{\partial z}{\partial y} = \dfrac{-y}{x + z}$

13. Verify the development of ∇^2 as given in Appendix V.

14. Given the function $u = 3x^2 + 2xz - y^2$, show that $x(\partial u/\partial x) + y(\partial u/\partial y) + z(\partial u/\partial z) = 2u$.

15. If $u = ln(x^2 + y^2)$, show that $(\partial^2 u/\partial x^2) + (\partial^2 u/\partial y^2) = 0$.

16. Show that $u = e^{-at} \cos bt$ is a solution to the equation $(\partial^2 u/\partial x^2) = (\partial u/\partial t)$, if the constants are chosen so that $a = b^2$.