

Clearly, the ideal gas law is suspect, but before concluding that the law is invalid in this situation, we should examine the data to see whether the error could be attributed to the experimental results. If so, we might be able to determine how much more accurate our experimental results would need to be to ensure that an error of this magnitude did not occur.

Analysis of the error involved in calculations is an important topic in numerical analysis and is introduced in Section 1.2. This particular application is considered in Exercise 28 of that section.

This chapter contains a short review of those topics from single-variable calculus that will be needed in later chapters. A solid knowledge of calculus is essential for an understanding of the analysis of numerical techniques, and more thorough review might be needed if you have been away from this subject for a while. In addition there is an introduction to convergence, error analysis, the machine representation of numbers, and some techniques for categorizing and minimizing computational error.

1.1 Review of Calculus

Limits and Continuity

The concepts of *limit* and *continuity* of a function are fundamental to the study of calculus, and form the basis for the analysis of numerical techniques.

Definition 1.1 A function f defined on a set X of real numbers has the **limit** L at x_0 , written

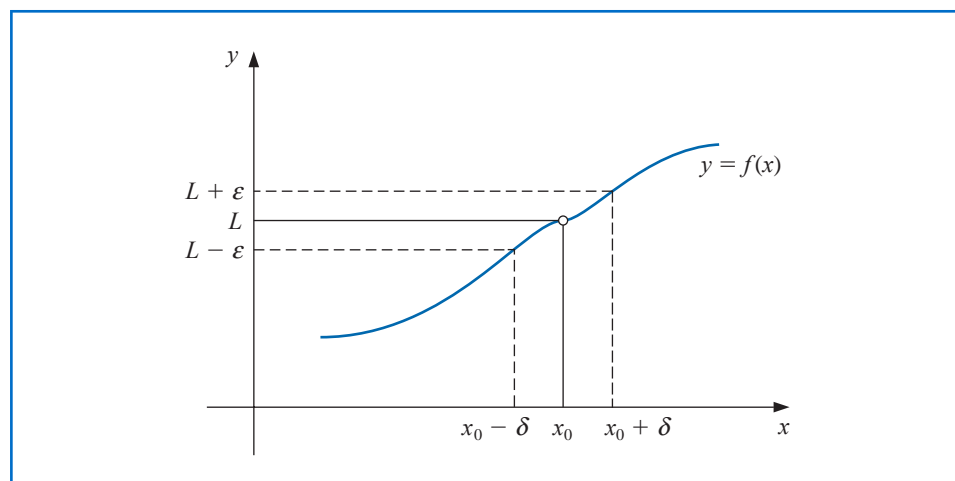
$$\lim_{x \rightarrow x_0} f(x) = L,$$

if, given any real number $\varepsilon > 0$, there exists a real number $\delta > 0$ such that

$$|f(x) - L| < \varepsilon, \quad \text{whenever } x \in X \quad \text{and} \quad 0 < |x - x_0| < \delta.$$

(See Figure 1.1.)

Figure 1.1



Definition 1.2

The basic concepts of calculus and its applications were developed in the late 17th and early 18th centuries, but the mathematically precise concepts of limits and continuity were not described until the time of Augustin Louis Cauchy (1789–1857), Heinrich Eduard Heine (1821–1881), and Karl Weierstrass (1815–1897) in the latter portion of the 19th century.

Let f be a function defined on a set X of real numbers and $x_0 \in X$. Then f is **continuous** at x_0 if

$$\lim_{x \rightarrow x_0} f(x) = f(x_0).$$

The function f is **continuous on the set X** if it is continuous at each number in X . ■

The set of all functions that are continuous on the set X is denoted $C(X)$. When X is an interval of the real line, the parentheses in this notation are omitted. For example, the set of all functions continuous on the closed interval $[a, b]$ is denoted $C[a, b]$. The symbol \mathbb{R} denotes the set of all real numbers, which also has the interval notation $(-\infty, \infty)$. So the set of all functions that are continuous at every real number is denoted by $C(\mathbb{R})$ or by $C(-\infty, \infty)$.

The *limit of a sequence* of real or complex numbers is defined in a similar manner.

Definition 1.3

Let $\{x_n\}_{n=1}^{\infty}$ be an infinite sequence of real numbers. This sequence has the **limit x (converges to x)** if, for any $\varepsilon > 0$ there exists a positive integer $N(\varepsilon)$ such that $|x_n - x| < \varepsilon$, whenever $n > N(\varepsilon)$. The notation

$$\lim_{n \rightarrow \infty} x_n = x, \quad \text{or} \quad x_n \rightarrow x \quad \text{as} \quad n \rightarrow \infty,$$

means that the sequence $\{x_n\}_{n=1}^{\infty}$ converges to x . ■

Theorem 1.4

If f is a function defined on a set X of real numbers and $x_0 \in X$, then the following statements are equivalent:

- a. f is continuous at x_0 ;
- b. If $\{x_n\}_{n=1}^{\infty}$ is any sequence in X converging to x_0 , then $\lim_{n \rightarrow \infty} f(x_n) = f(x_0)$. ■

The functions we will consider when discussing numerical methods will be assumed to be continuous because this is a minimal requirement for predictable behavior. Functions that are not continuous can skip over points of interest, which can cause difficulties when attempting to approximate a solution to a problem.

Differentiability

More sophisticated assumptions about a function generally lead to better approximation results. For example, a function with a smooth graph will normally behave more predictably than one with numerous jagged features. The smoothness condition relies on the concept of the derivative.

Definition 1.5

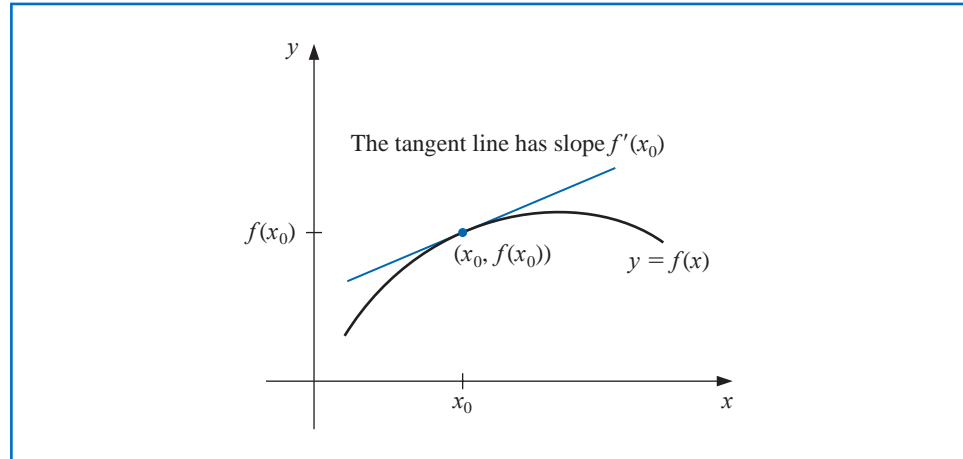
Let f be a function defined in an open interval containing x_0 . The function f is **differentiable** at x_0 if

$$f'(x_0) = \lim_{x \rightarrow x_0} \frac{f(x) - f(x_0)}{x - x_0}$$

exists. The number $f'(x_0)$ is called the **derivative** of f at x_0 . A function that has a derivative at each number in a set X is **differentiable on X** . ■

The derivative of f at x_0 is the slope of the tangent line to the graph of f at $(x_0, f(x_0))$, as shown in Figure 1.2.

Figure 1.2



Theorem 1.6 If the function f is differentiable at x_0 , then f is continuous at x_0 . ■

The theorem attributed to Michel Rolle (1652–1719) appeared in 1691 in a little-known treatise entitled *Méthode pour résoudre les égalités*. Rolle originally criticized the calculus that was developed by Isaac Newton and Gottfried Leibniz, but later became one of its proponents.

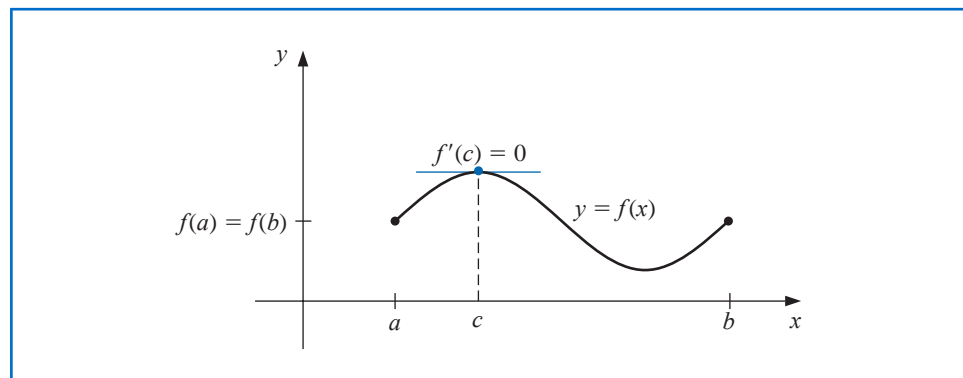
The next theorems are of fundamental importance in deriving methods for error estimation. The proofs of these theorems and the other unreferenced results in this section can be found in any standard calculus text.

The set of all functions that have n continuous derivatives on X is denoted $C^n(X)$, and the set of functions that have derivatives of all orders on X is denoted $C^\infty(X)$. Polynomial, rational, trigonometric, exponential, and logarithmic functions are in $C^\infty(X)$, where X consists of all numbers for which the functions are defined. When X is an interval of the real line, we will again omit the parentheses in this notation.

Theorem 1.7 (Rolle's Theorem)

Suppose $f \in C[a, b]$ and f is differentiable on (a, b) . If $f(a) = f(b)$, then a number c in (a, b) exists with $f'(c) = 0$. (See Figure 1.3.) ■

Figure 1.3

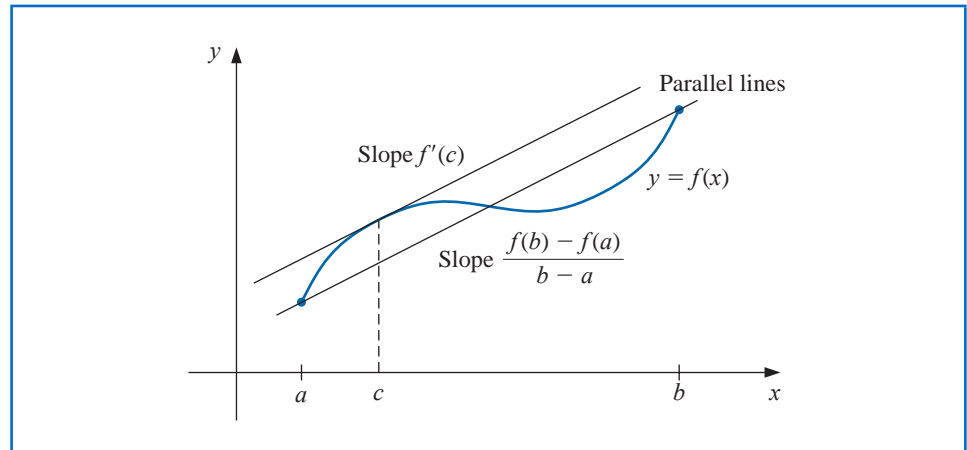


Theorem 1.8 (Mean Value Theorem)

If $f \in C[a, b]$ and f is differentiable on (a, b) , then a number c in (a, b) exists with (See Figure 1.4.)

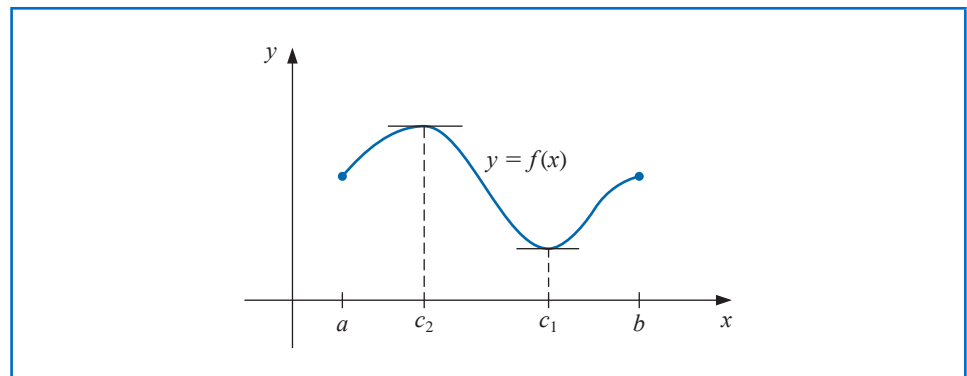
$$f'(c) = \frac{f(b) - f(a)}{b - a}. \quad \blacksquare$$

Figure 1.4

**Theorem 1.9 (Extreme Value Theorem)**

If $f \in C[a, b]$, then $c_1, c_2 \in [a, b]$ exist with $f(c_1) \leq f(x) \leq f(c_2)$, for all $x \in [a, b]$. In addition, if f is differentiable on (a, b) , then the numbers c_1 and c_2 occur either at the endpoints of $[a, b]$ or where f' is zero. (See Figure 1.5.) ■

Figure 1.5



Research work on the design of algorithms and systems for performing symbolic mathematics began in the 1960s. The first system to be operational, in the 1970s, was a LISP-based system called MACSYMA.

As mentioned in the preface, we will use the computer algebra system Maple whenever appropriate. Computer algebra systems are particularly useful for symbolic differentiation and plotting graphs. Both techniques are illustrated in Example 1.

Example 1 Use Maple to find the absolute minimum and absolute maximum values of

$$f(x) = 5 \cos 2x - 2x \sin 2x$$

on the intervals **(a)** $[1, 2]$, and **(b)** $[0.5, 1]$

Solution There is a choice of Text input or Math input under the Maple C 2D Math option. The Text input is used to document worksheets by adding standard text information in the document. The Math input option is used to execute Maple commands. Maple input

The Maple development project began at the University of Waterloo in late 1980. Its goal was to be accessible to researchers in mathematics, engineering, and science, but additionally to students for educational purposes. To be effective it needed to be portable, as well as space and time efficient. Demonstrations of the system were presented in 1982, and the major paper setting out the design criteria for the MAPLE system was presented in 1983 [CGGG].

can either be typed or selected from the pallets at the left of the Maple screen. We will show the input as typed because it is easier to accurately describe the commands. For pallet input instructions you should consult the Maple tutorials. In our presentation, Maple input commands appear in *italic* type, and Maple responses appear in cyan type.

To ensure that the variables we use have not been previously assigned, we first issue the command.

restart

to clear the Maple memory. We first illustrate the graphing capabilities of Maple. To access the graphing package, enter the command

with(plots)

to load the plots subpackage. Maple responds with a list of available commands in the package. This list can be suppressed by placing a colon after the *with(plots)* command.

The following command defines $f(x) = 5 \cos 2x - 2x \sin 2x$ as a function of x .

$f := x \rightarrow 5 \cos(2x) - 2x \cdot \sin(2x)$

and Maple responds with

$$x \rightarrow 5 \cos(2x) - 2x \sin(2x)$$

We can plot the graph of f on the interval $[0.5, 2]$ with the command

plot(f, 0.5 . . 2)

Figure 1.6 shows the screen that results from this command after doing a mouse click on the graph. This click tells Maple to enter its graph mode, which presents options for various views of the graph. We can determine the coordinates of a point of the graph by moving the mouse cursor to the point. The coordinates appear in the box above the left of the *plot(f, 0.5 . . 2)* command. This feature is useful for estimating the axis intercepts and extrema of functions.

The absolute maximum and minimum values of $f(x)$ on the interval $[a, b]$ can occur only at the endpoints, or at a critical point.

(a) When the interval is $[1, 2]$ we have

$$f(1) = 5 \cos 2 - 2 \sin 2 = -3.899329036 \quad \text{and} \quad f(2) = 5 \cos 4 - 4 \sin 4 = -0.241008123.$$

A critical point occurs when $f'(x) = 0$. To use Maple to find this point, we first define a function *fp* to represent f' with the command

$fp := x \rightarrow \text{diff}(f(x), x)$

and Maple responds with

$$x \rightarrow \frac{d}{dx} f(x)$$

To find the explicit representation of $f'(x)$ we enter the command

fp(x)

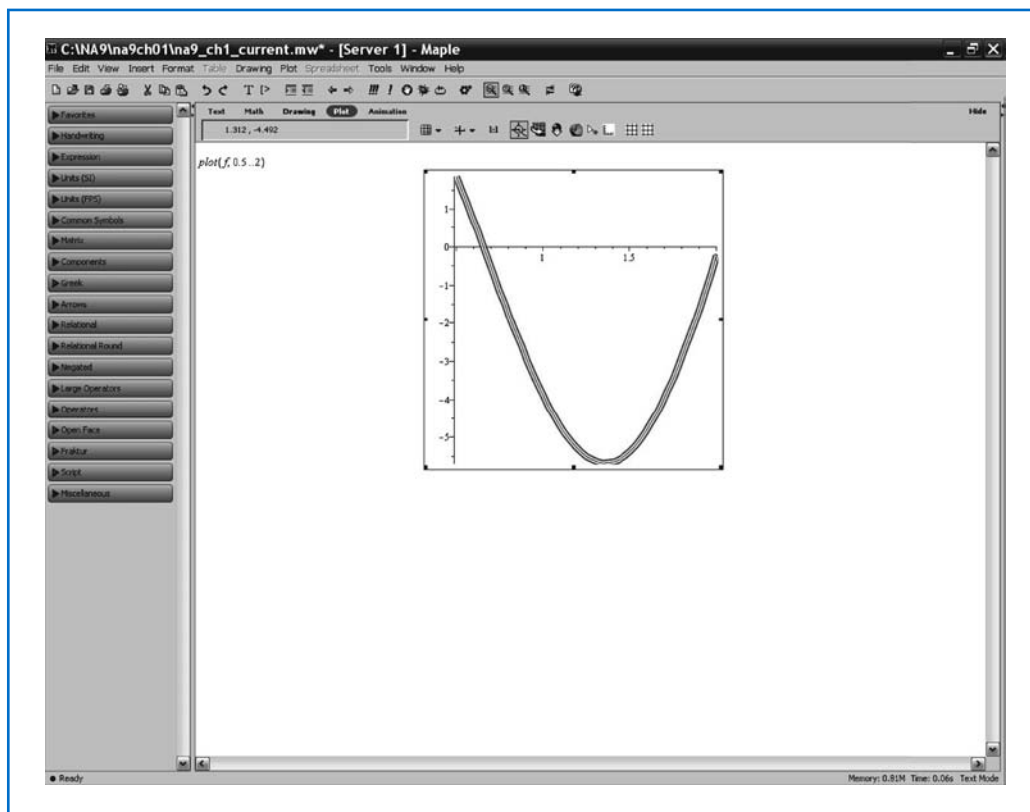
and Maple gives the derivative as

$$-12 \sin(2x) - 4x \cos(2x)$$

To determine the critical point we use the command

fsolve(fp(x), x, 1 . . 2)

Figure 1.6



and Maple tells us that $f'(x) = fp(x) = 0$ for x in $[1, 2]$ when x is

$$1.358229874$$

We evaluate $f(x)$ at this point with the command

$f(\%)$

The $\%$ is interpreted as the last Maple response. The value of f at the critical point is

$$-5.675301338$$

As a consequence, the absolute maximum value of $f(x)$ in $[1, 2]$ is $f(2) = -0.241008123$ and the absolute minimum value is $f(1.358229874) = -5.675301338$, accurate at least to the places listed.

(b) When the interval is $[0.5, 1]$ we have the values at the endpoints given by

$$f(0.5) = 5 \cos 1 - 1 \sin 1 = 1.860040545 \quad \text{and} \quad f(1) = 5 \cos 2 - 2 \sin 2 = -3.899329036.$$

However, when we attempt to determine the critical point in the interval $[0.5, 1]$ with the command

$fsolve(fp(x), x, 0.5 . . 1)$

Maple gives the response

$$fsolve(-12 \sin(2x) - 4x \cos(2x), x, .5 . . 1)$$

This indicates that Maple is unable to determine the solution. The reason is obvious once the graph in Figure 1.6 is considered. The function f is always decreasing on this interval, so no solution exists. Be suspicious when Maple returns the same response it is given; it is as if it was questioning your request.

In summary, on $[0.5, 1]$ the absolute maximum value is $f(0.5) = 1.86004545$ and the absolute minimum value is $f(1) = -3.899329036$, accurate at least to the places listed. ■

The following theorem is not generally presented in a basic calculus course, but is derived by applying Rolle's Theorem successively to f , f' , \dots , and, finally, to $f^{(n-1)}$. This result is considered in Exercise 23.

Theorem 1.10 (Generalized Rolle's Theorem)

Suppose $f \in C[a, b]$ is n times differentiable on (a, b) . If $f(x) = 0$ at the $n + 1$ distinct numbers $a \leq x_0 < x_1 < \dots < x_n \leq b$, then a number c in (x_0, x_n) , and hence in (a, b) , exists with $f^{(n)}(c) = 0$. ■

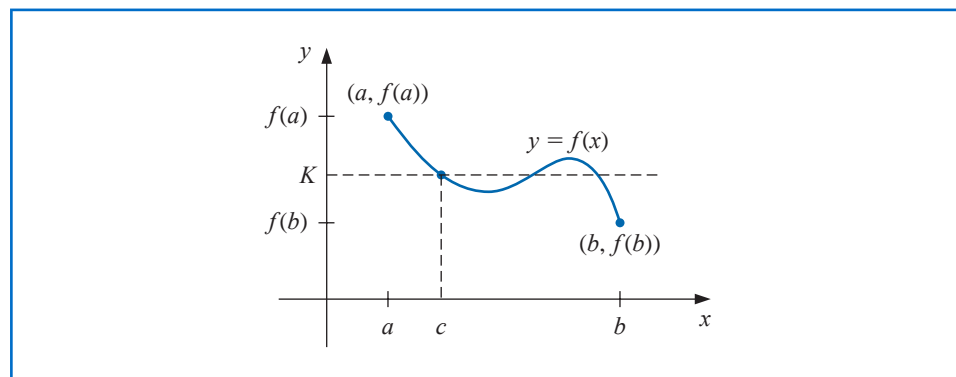
We will also make frequent use of the Intermediate Value Theorem. Although its statement seems reasonable, its proof is beyond the scope of the usual calculus course. It can, however, be found in most analysis texts.

Theorem 1.11 (Intermediate Value Theorem)

If $f \in C[a, b]$ and K is any number between $f(a)$ and $f(b)$, then there exists a number c in (a, b) for which $f(c) = K$. ■

Figure 1.7 shows one choice for the number that is guaranteed by the Intermediate Value Theorem. In this example there are two other possibilities.

Figure 1.7



Example 2 Show that $x^5 - 2x^3 + 3x^2 - 1 = 0$ has a solution in the interval $[0, 1]$.

Solution Consider the function defined by $f(x) = x^5 - 2x^3 + 3x^2 - 1$. The function f is continuous on $[0, 1]$. In addition,