```
    336*exp(x)/x^4 + 1680*exp(x)/x^5 -
      6720*exp(x)/x^6 + 20160*exp(x)/x^7 -
        40320*exp(x)/x^8 + 40320*exp(x)/x^9
```

The expression for the eighth derivative is pretty complicated. We can get the numerical values of these at $x = 3$:

```
EDU>> numeric(subs (df2, 3))
  ans =
    3.7195
EDU>> numeric(subs (df8, 3))
  ans =
    3.7563
```

Extrapolation Techniques

We found earlier that the errors of a central-difference approximation to $f'(x)$ were of $O(h^2)$. In effect, that suggests that the errors are proportional to h^2 although that is true only in the limit as $h \to 0$. Unless h is quite large, we can assume the proportionality. So, from two computations with h being half as large in the second, we can estimate the proportionality factor which we call C. For example, in Table 5.2 we had:

h	Approximation
0.05	4.15831
0.025	4.16361

If errors were truly $C(h^2)$, we can write two equations:

$$\text{True value} = 4.15831 + C(0.05^2)$$
$$\text{True value} = 4.16361 + C(0.025^2)$$

from which we can solve for the true value, eliminating the unknown "constant" C, getting:

$$\begin{aligned}\text{True value} &= 4.16361 + (1/3) * (4.16361 - 4.15831)\\ &= 4.16538,\end{aligned}$$

which is very close to the exact value for $f'(1.9)$, 4.165382.

You can easily derive the general formula for improving the estimate, when errors decrease by $O(h^n)$:

$$\underset{\text{estimate}}{\text{Better}} = \underset{\text{accurate}}{\text{more}} + (1/(2^n - 1))(\text{more} - \text{less}), \tag{5.15}$$

where more and less in the last term are the two estimates at h_1 and $h_2 = h_1/2$. "More accurate" is the estimate at the smaller value of h and n is the power of h in the order of the errors.

As a second example, let us apply this to values from Table 5.1 which were from forward-difference approximations. Here the errors are $O(h)$.

```
xp(x)/x^4 + 1680*exp(x)/x^5 –
0*exp(x)/x^6 + 20160*exp(x)/x^7 –
40320*exp(x)/x^8 + 40320*exp(x)/x^9
```

the eighth derivative is pretty complicated. We can get the
= 3:

```
ic(subs (df2, 3))
```

```
ic(subs (df8, 3))
```

n Techniques

hat the errors of a central-difference approximation to $f'(x)$ were
t suggests that the errors are proportional to h^2 although that is true
0. Unless h is quite large, we can assume the proportionality. So, fi
with h being half as large in the second, we can estimate the propo
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	oproximation
	4.15831
	4.16361

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$$\text{True value} = 4.15831 + C(0.05^2)$$
$$\text{True value} = 4.16361 + C(0.025^2)$$

solve for the true value, eliminating the unknown "constant" C, getting

$$\text{True value} = 4.16361 + (1/3) * (4.16361 - 4.15831)$$
$$= 4.16538,$$

to the exact value for $f'(1.9)$, 4.165382.
derive the general formula for improving the estimate, when error

$$\text{Better estimate} = \text{more accurate} + (1/(2^n - 1))(\text{more} - \text{less}), \quad (5.15)$$

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at the smaller value of h and n is the power of h in the order of the error
ample, let us apply this to values from Table 5.1 which were from h
proximations. Here the errors are $O(h)$.

h	Approximation
0.05	4.05010
0.025	4.10955

Using Eq. (5.15), we have

$$\text{Better estimate} = 4.10955 + (4.10955 - 4.05010)\,(1/(2^1 - 1))$$
$$= 4.16900,$$

which shows considerable improvement but not as good as from the central differences.

This extrapolation technique applies to any set of computations where the order of the error is known, and we will see later in this chapter that we can apply it to integration methods. Of course it also applies to the computation of higher derivatives, such as from Eq. (5.14).

Richardson Extrapolation

When we compute an extrapolation from two estimates of the derivative using, say, $h = 0.1$ and $h = 0.05$, both of which are of $O(h^2)$, the improved estimate has an error $O(h^4)$ as we show below. If we do another computation of $f'(x)$ at $h = 0.025$ to get a third estimate of $f'(x)$ and use this with the estimate at $h = 0.05$ to extrapolate, we get a second further improved estimate also of error $O(h^4)$. What is the error if we use these two improved estimates to extrapolate again?

Consider the difference between the pair of Taylor series that gave rise to Eq. (5.3) but with more terms:

$$f_i' = (f(x + h) - f(x - h))/(2h) + a_1h^2 + a_2h^4 + a_3h^6 + \cdots. \quad (5.16)$$

(The terms on the right after the first represent the error of the central difference approximation; the odd powers of h drop out through cancellations.)

If we compute a second approximation for f_i' but with h cut in half, we get a better approximation:

$$f_i' = (f(x + h/2) - f(x - h/2))/(h) + a_1h^2/4 + a_2h^4/16 + a_3h^6/64 + \cdots. \quad (5.17)$$

Adding 1/3 of the difference between Eqs. (5.17) and (5.16) to Eq. (5.17) gives Eq. (5.15), but now we see that n will be 4 because the first of the errors terms cancel.

Using the two improved estimates for the derivative, but now adding 1/15 of the difference to the better estimate, results in canceling the next error term; it will be of $O(h^6)$. Continuing in the same fashion gives estimates of $O(h^8)$, $O(h^{10})$, . . . , until there is no change in the improvements. Doing these successive extrapolations is called *Richardson extrapolation.*

Here is an example with $f(x) = x^2 * \cos(x)$ for which $f(1.0) = 0.23913363$. The original values of $f'(1.0)$ are from central differences so they are of $O(h^2)$.

Value of h	$f'(1.0)$	First extrapolations	Second extrapolations	Third extrapolations
0.1	0.226736			
0.05	0.236031	0.239129		
0.025	0.238258	0.239133	0.239134	
0.0125	0.238940	0.239132	0.239132	0.239132

There really was no point in doing the third extrapolation because the second one did not change the value.

The merit of Richardson extrapolation is that we get greatly improved estimates without having to evaluate the function additional times. We can use this technique to extrapolate higher derivatives as well.

An Algorithm to Compute a Richardson Table That Computes the Derivative, f′(x)

Given a function $f(x)$:

Input
  x = value for x
  h = starting value for stepsize h
  MaxStage = maximum number of stages (lines of table)
  Tol = tolerance value for termination
  $d(0, 1) = 0$: the initial value of the table

(Compute lines, (stages) of the table)
  For stage = 1 To MaxStage Step 1 Do
    Set $d(\text{stage}, 1) = [f(x + h) - f(x - h)]/(2h)$.
    For j = 2 to stage Step 1 Do
      Set $d(\text{stage}, j) = d(\text{stage}, j - 1)$
        $+ [d(\text{stage}, j - 1) - d(\text{stage} - 1, j - 1)]/(2^{2j} - 1)$
    EndDo (For j).
    If $|d(\text{stage}, \text{stage}) - d(\text{stage}, \text{stage} - 1)| < \text{Tol}$
    Then Exit EndIf.
    Set $h = h/2$
  EndDo (For stage).

On termination, the last computed value is the extrapolated estimate of the derivative.

Extrapolation with Tabulated Values

If we only have an evenly spaced table of $(x, f(x))$ values, as we might have from a set of experiments, we have no way to get new function values where the differences in x are halved. However, if there are enough entries in the table, we may be able to double the Δx's. Table 5.5 is an example.

First extrapolations	Second extrapolations	Third extrapolati
0.239129		
0.239133	0.239134	
0.239132	0.239132	0.23913

nt in doing the third extrapolation because the second one did no

on extrapolation is that we get greatly improved estimates witho
unction additional times. We can use this technique to extrapola
1.

ute a Richardson
he Derivative, f′(x)

for stepsize h
mum number of stages (lines of table)
lue for termination
itial value of the table

es) of the table)
MaxStage Step 1 Do
$= [f(x + h) - f(x - h)]/(2h)$.
ge Step 1 Do
$j) = d(\text{stage}, j - 1)$
$\text{ge}, j - 1) - d(\text{stage} - 1, j - 1)]/(2^{2j} - 1)$

$\text{e}) - d(\text{stage}, \text{stage} - 1)| < \text{Tol}$
f.

ast computed value is the extrapolated estimate of the derivative.

ith Tabulated Values

ly spaced table of $(x, f(x))$ values, as we might have from a set of
no way to get new function values where the differences in x are
re are enough entries in the table, we may be able to double the
ample.

Table 5.5

i	x_i	f_i
0	2.0	0.123060
1	2.1	0.105706
2	2.2	0.089584
3	2.3	0.074764
4	2.4	0.061277
5	2.5	0.049126
6	2.6	0.038288
7	2.7	0.028722
8	2.8	0.020371
9	2.9	0.013164
10	3.0	0.007026

Suppose we want the derivative at $x = 2.4$. The central difference approximation is -0.12819 from $f(2.3)$ and $f(2.5)$, $h = 0.1$. Now, if we compute the value again, but use the values at $x = 2.2$ and 2.6, where $h = 0.2$, we get -0.12824, a poorer estimate because h is twice as large. However, since we known that both are of $O(h^2)$, we can employ Eq. (5.15) to get an improvement:

$$\begin{aligned} f'(2.4)\ [\text{improved}] &= -0.12819 + (-0.12819 + 0.12824)/3 \\ &= -0.12817. \end{aligned}$$

[The function in Table 5.5 is for $f(x) = e^{-x}\sin(x)$ for, which $f'(2.4) = -0.128171$.]

For convenience, here we collect formulas for computing derivatives.

Formulas for Computing Derivatives

Formulas for the first derivative:

$$f'(x_0) = \frac{f_1 - f_0}{h} + O(h)$$

$$f'(x_0) = \frac{f_1 - f_{-1}}{2h} + O(h^2) \qquad \text{Central difference}$$

$$f'(x_0) = \frac{-f_2 - 4f_1 - 3f_0}{2h} + O(h^2)$$

$$f'(x_0) = \frac{-f_2 + 8f_1 - 8f_{-1} + f_{-2}}{12h} + O(h^4) \qquad \text{Central difference}$$

Formulas for the second derivative:

$$f''(x_0) = \frac{f_2 - 2f_1 + f_0}{h^2} + O(h)$$

$$f''(x_0) = \frac{f_1 - 2f_0 + f_{-1}}{h^2} + O(h^2) \qquad \text{Central difference}$$

$$f''(x_0) = \frac{-f_3 + 4f_2 - 5f_1 + 2f_0}{h^2} + O(h^2)$$

$$f''(x_0) = \frac{-f_2 + 16f_1 - 30f_0 + 16f_{-1} - f_{-2}}{12h^2} + O(h^4) \qquad \text{Central difference}$$

Formulas for the third derivative:

$$f'''(x_0) = \frac{f_3 - 3f_2 + 3f_1 - f_0}{h^3} + O(h)$$

$$f'''(x_0) = \frac{f_2 - 2f_1 + 2f_{-1} - f_{-2}}{2h^3} + O(h^2) \qquad \text{Averaged difference}$$

Formulas for the fourth derivative:

$$f^{\text{iv}}(x_0) = \frac{f_4 - 4f_3 + 6f_2 - 4f_1 + f_0}{h^4} + O(h)$$

$$f^{\text{iv}}(x_0) = \frac{f_2 - 4f_1 + 6f_0 - 4f_{-1} + f_{-2}}{h^4} + O(h^2) \qquad \text{Central difference}$$

5.2 Numerical Integration—The Trapezoidal Rule

Integral calculus is a most important branch of calculus. It is used to find the velocity of a body when its acceleration is known, to find the distance traveled using the velocity, to compute areas, to predict population growth, and in many other important applications.

In your calculus course, you learned many formulas to get the *indefinite integral* of function $f(x)$, the *antiderivative.* [Given the function, $f(x)$, the antiderivative is a function $F(x)$ such that $F'(x) = f(x)$.] You learned that the *definite integral,*

$$\int_a^b f(x) = F(b) - F(a),$$

can be evaluated from the antiderivative. Still, there are functions that do not have an antiderivative expressible in terms of ordinary functions.

All of our computer algebra systems can find the antiderivative if its table of integrals has it. For example, in Maple,

```
>int(x*sin(x), x);
   sin(x) - x cos(x)
```

but, if the antiderivative in unknown, it just returns $\int f(x)\,dx$:

$\frac{\ldots + f_{-1}}{\ldots^2} + O(h^2)$ Central difference

$\frac{4f_2 - 5f_1 + 2f_0}{h^2} + O(h^2)$

$\frac{16f_1 - 30f_0 + 16f_{-1} - f_{-2}}{12h^2} + O(h^4)$ Central difference

ird derivative:

$\frac{f_2 + 3f_1 - f_0}{h^3} + O(h)$

$\frac{f_1 + 2f_{-1} - f_{-2}}{2h^3} + O(h^2)$ Averaged difference

urth derivative:

$\frac{f_3 + 6f_2 - 4f_1 + f_0}{h^4} + O(h)$

$\frac{f_1 + 6f_0 - 4f_{-1} + f_{-2}}{h^4} + O(h^2)$ Central difference

egration – The Trapezoidal Rule

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$$\int_a^b f(x) = F(b) - F(a),$$

e antiderivative. Still, there are functions that do not have an anti
terms of ordinary functions.
algebra systems can find the antiderivative if its table of integrals
aple,

```
x);
x)
```

in unknown, it just returns $\int f(x)\,dx$:

$$\int \frac{e^x}{\ln(x)}\,dx$$

If we give limits for the integral,

```
>int(x*sin(x), x=1..2);
  sin(2) - 2 cos(2) - sin(1) + cos(1)
```

Maple gives us $F(b) - F(a)$, which we can evaluate with

```
>evalf(%)
  1.440422421
```

Now we ask, "Is there any way that the definite integral can be found when the antiderivative is unknown?" The answer is "Yes, we can do it numerically."

You learned that the definite integral is the area between the curve of $f(x)$ and the x-axis. That is the principle behind all numerical integration—we divide the distance from $x = a$ to $x = b$ into vertical strips and add the areas of these strips (the strips are often made equal in widths but that is not always required).

The Trapezoidal Rule

When the area between the curve of $f(x)$ and the x-axis is subdivided into strips, one way to draw the strips is to make the top of the strips touch the curve, either at the left corner or the right corner, but that is less accurate than making the top of the strip even with the curve at its midpoint. In effect, these schemes replace the curve for $f(x)$ with a sequence of horizontal lines. We can think of these lines as interpolating polynomials of degree zero.

A much better way is to approximate the curve with a sequence of straight lines; in effect, we slant the top of the strips to match with the curve as best we can. We are approximating the curve with interpolating polynomials of degree-1. The gives us the *trapezoidal rule.* Figure 5.2 illustrates this.

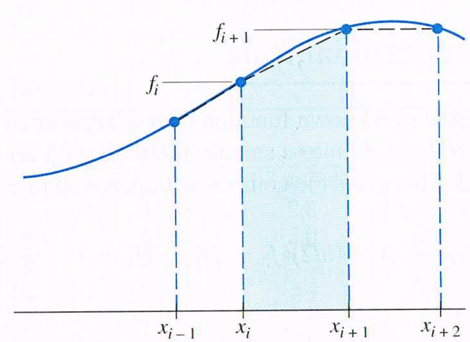

Figure 5.2

From Figure 5.2, it is intuitively clear that the area of the strip from x_i to x_{i+1} gives an approximation to the area under the curve:

$$\int_{x_i}^{x_{i+1}} f(x)\,dx \approx \frac{f_i + f_{i+1}}{2}(x_{i+1} - x_i).$$

We will usually write $h = (x_{i+1} - x_i)$ for the width of the interval.

Another Derivation of the Trapezoidal Rule

An alternative way to obtain the trapezoidal rule is to fit $f(x)$ between pairs of x-values with polynomials of degree-1 and integrate those polynomials. We learned in Chapter 3 that the first-degree Newton–Gregory interpolating polynomial between points x_i and x_{i+1} was

$$f(x) \approx P_1(x) = f_i + s\Delta f_i + \text{error},$$

where $s = (x - x_i)/h$ and the error is given by

$$(h^2/2)(s)(s-1)f''(\xi).$$

We can estimate $\int f(x)$ between the two points by integrating $P_1(x)$:

$$\int_{x_i}^{x_{i+1}} f(x)\,dx \approx \int_{x_i}^{x_{i+1}} P_1(x) = \int_{x_i}^{x_{i+1}} (f_i + s\Delta f_i)\,dx = h\int_0^1 (f_i + s\Delta f_i)\,ds,$$

where we have replaced dx with $h * ds$, and noted that $s = 0$ at x_i and $s = 1$ at x_{i+1}.
Carrying out the integration, we find that

$$\int_{x_i}^{x_{i+1}} f(x)\,dx \approx \int_{x_i}^{x_{i+1}} P_1(x) = h(f_i + (1/2)\Delta f_i) = (h/2)(f_i + f_{i+1}),$$

exactly as we found intuitively. The real reason for this development is to find the error term for one application of trapezoidal integration. We get this by integrating the error term. Doing so, we find

$$\text{Error} = -(1/12)h^3 f'''(\xi) = O(h^3).$$

The Composite Trapezoidal Rule

If we are getting the integral of a known function over a larger span of x-values, say, from $x = a$ to $x = b$, we subdivide $[a, b]$ into n smaller intervals with $\Delta x = h$, apply the rule to each subinterval, and add. This gives the composite trapezoidal rule:

$$\int_a^b f(x)\,dx \approx \sum_{i=0}^{n-1} (h/2)(f_i + f_{i+1}) = (h/2)(f_0 + 2f_1 + 2f_2 + \cdots + 2f_{n-1} + f_n). \quad \text{(5.18)*}$$

* In a computer program, you should do $h(f_0/2 + f_1 + f_2 + \cdots + f_{n-1} + f_n/2)$ in order to reduce the number of operations.

...area under the curve:

$$\int_{x_i}^{x_{i+1}} f(x)\,dx \approx \frac{f_i + f_{i+1}}{2}(x_{i+1} - x_i).$$

...$h = (x_{i+1} - x_i)$ for the width of the interval.

...ation of the Trapezoidal Rule

...obtain the trapezoidal rule is to fit $f(x)$ between pairs of x-values ...ee-1 and integrate those polynomials. We learned in Chapter ... Gregory interpolating polynomial between points x_i and x_{i+1} ...

$$f(x) \approx P_1(x) = f_i + s\Delta f_i + \text{error},$$

and the error is given by

$$(h^2/2)(s)(s-1)f''(\xi).$$

... between the two points by integrating $P_1(x)$:

$$\approx \int_{x_i}^{x_{i+1}} P_1(x) = \int_{x_i}^{x_{i+1}} (f_i + s\Delta f_i)\,dx = h\int_0^1 (f_i + s\Delta f_i)\,ds,$$

...ed dx with $h * ds$, and noted that $s = 0$ at x_i and $s = 1$ at x_{i+1}, ...tegration, we find that

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...Trapezoidal Rule

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$$\ldots f_i + f_{i+1}) = (h/2)(f_0 + 2f_1 + 2f_2 + \cdots + 2f_{n-1} + f_n). \quad (5.10)$$

...u should do $h(f_0/2 + f_1 + f_2 + \cdots + f_{n-1} + f_n/2)$ in order to reduce the number of ...

The error now is not the *local error* $O(h^3)$ but the *global error,* the sum of n local errors:

$$\text{Global error} = (-1/12)h^3[f''(\xi_1) + f''(\xi_2) + \cdots + f''(\xi_n)].$$

In this equation, each of the ξ_i is somewhere within each subinterval. If $f''(x)$ is continuous in $[a, b]$, there is some point within $[a, b]$ at which the sum of the $f''(\xi_i)$ is equal to $f''(\xi)$, where ξ is in $[a, b]$. We then see that, because $nh = (b - a)$,

$$\text{Global error} = (-1/12)h^3 nf''(\xi) = \frac{-(b-a)}{12}h^2 f''(\xi) = O(h^2).$$

The fact that the global error is $O(h^2)$ while the local error is $O(h^3)$ seems reasonable because, for example, if we double the number of subintervals, we add together twice as many local errors.

EXAMPLE 5.1 Given the values for x and $f(x)$ in Table 5.6, use the trapezoidal rule to estimate the integral from $x = 1.8$ to $x = 3.4$.

Applying the trapezoidal rule:

$$\int_{1.8}^{3.4} f(x)\,dx \approx \frac{0.2}{2}[6.050 + 2(7.389) + 2(9.025) + 2(11.023) + 2(13.464)$$
$$+ 2(16.445) + 2(20.086) + 2(24.533) + 29.964] = 23.9944.$$

The data in Table 5.6 are for $f(x) = e^x$ and the true value is $e^{3.4} - e^{1.8} = 23.9144$. The trapezoidal rule value is off by 0.08; there are three digits of accuracy. How does this compare to the estimated error?

$$\text{Error} = -\frac{1}{12}h^3 nf''(\xi), \qquad 1.8 \le \xi \le 3.4,$$

$$= -\frac{1}{12}(0.2)^3(8) * \begin{Bmatrix} e^{1.8} & (\max) \\ e^{3.4} & (\min) \end{Bmatrix} = \begin{Bmatrix} -0.0323 & (\max) \\ -0.1598 & (\min) \end{Bmatrix}.$$

Table 5.6

x	$f(x)$	x	$f(x)$
1.6	4.953	2.8	16.445
1.8	6.050	3.0	20.086
2.0	7.389	3.2	24.533
2.2	9.025	3.4	29.964
2.4	11.023	3.6	36.598
2.6	13.464	3.8	44.701

Alternatively,

$$\text{Error} = -\frac{1}{12}(0.2)^2(3.4 - 1.8)*\begin{Bmatrix} e^{1.8} & (\max) \\ e^{3.4} & (\min) \end{Bmatrix} = \begin{Bmatrix} -0.0323 \\ -0.1598 \end{Bmatrix}.$$

The actual error was −0.080.

If we had not known the function for which we have tabulated values, we would have estimated $h^2 f''(\xi)$ from the second differences.

An Algorithm for Integration by the Composite Trapezoidal Rule

Given a function $f(x)$:

(Get user inputs).
Input
 a, b = endpoints of interval
 n = number of intervals

(Do the integration)
Set $h = (b - a)/n$.
Set sum = 0
For $i = 1$ to $n - 1$ Step 1 Do
 Set $x = a + h * i$,
 Set sum = sum + 2 * $f(x)$
End Do (For i).
Set sum = sum + $f(a) + f(b)$.
Set ans = sum * $h/2$.

The value of the integral is given by ans.

Unevenly Spaced Data

Data from experimental observations may not be evenly spaced. The trapezoidal rule still applies. Suppose there are five points:

$$\int f(x) \approx \frac{f_0 + f_1}{2}(x_1 - x_0) + \frac{f_1 + f_2}{2}(x_2 - x_1) + \frac{f_2 + f_3}{2}(x_3 - x_2) + \frac{f_3 + f_4}{2}(x_4 - x_3)$$
$$= \sum_{i=0}^{3} \frac{f_i + f_{i+1}}{2}(x_{i+1} - x_i).$$

There is no simple way to express this.

Romberg Integration

We can improve the accuracy of the trapezoidal rule integral by a technique that is similar

$$-\frac{1}{12}(0.2)^2(3.4 - 1.8)*\begin{Bmatrix} e^{1.8} & (\max) \\ e^{3.4} & (\min) \end{Bmatrix} = \begin{Bmatrix} -0.0323 \\ -0.1598 \end{Bmatrix}.$$

$-0.080.$

wn the function for which we have tabulated values, we would h
m the second differences.

ntegration by the Composite Trapezoidal Rule

$f(x)$:

ts of interval
of intervals

n)

Step 1 Do
* i,
n + 2 * $f(x)$

$f(a) + f(b)$.
$/2$.

ntegral is given by ans.

ced Data

ntal observations may not be evenly spaced. The trapezoidal rule
re are five points:

$$- x_0) + \frac{f_1 + f_2}{2}(x_2 - x_1) + \frac{f_2 + f_3}{2}(x_3 - x_2) + \frac{f_3 + f_4}{2}(x_4$$

$$(x_{i+1} - x_i).$$

ay to express this.

gration

accuracy of the trapezoidal rule integral by a technique that is simil

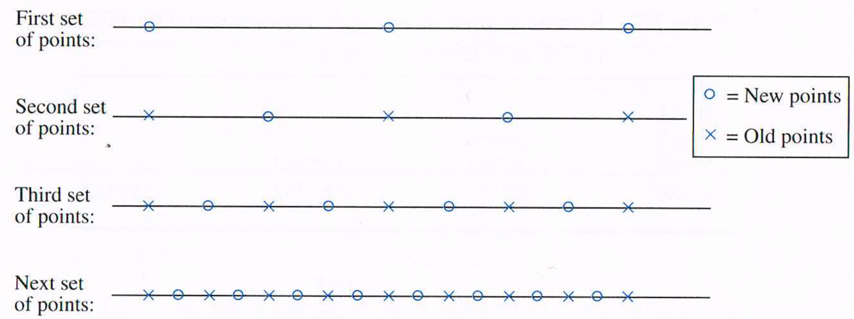

Figure 5.3

Because the integral determined with the trapezoidal method has an error of $O(h^2)$, we can combine two estimates of the integral that have h-values in a 2:1 ratio by Eq. (5.15), which we repeat here:

$$\text{Better estimate} = \text{more accurate} + \frac{1}{2^n - 1}(\text{more accurate} - \text{less accurate}).* \qquad \textbf{(5.19)}$$

When we apply this equation to get the integral of a known function, we begin with an arbitrary value for h in Eq. (5.18). A second estimate is then made with the value of h halved. From these two estimates we extrapolate to get an improved estimate using Eq. (5.19). This has an error of $O(h^4)$.

Obviously, this can be extended to produce a table of successively better estimates. When we find that the values converge, we have the best estimate that we can make in the light of round-off error. As shown before, each new extrapolation has error orders that increase: $O(h^4)$, $O(h^6)$, $O(h^8)$, ...

We can reduce the number of computations because, when h is halved, all of the old points at which the function was evaluated to get Eq. (5.18) appear in the new computation and we thus can avoid repeating the evaluations. Figure 5.3 illustrates this point.

This next example shows how the *Romberg table* appears for the function $f(x) = e^{-x^2}$ integrated between the limits of 0.2 and 1.5. This integral has no closed form solution. It is closely related to the *error function,* a quantity that is so important in statistics and other branches of applied mathematics that values have been tabulated.

EXAMPLE 5.2 Use Romberg integration to find the integral of e^{-x^2} between the limits of $a = 0.2$ and $b = 1.5$. Take the initial subinterval size as $h = (b - a)/2 = 0.65$.

Our first estimate is

$$\text{Integral} = \frac{h}{2}[f(a) + 2f(a + h) + f(b)]$$

* In Eq. (5.19), n is the order of the error. In the first extrapolation, $n = 2$. In successive extrapolations, it

Table 5.7 Romberg table of integrals over interval from 0.2 to 1.5 with an initial h of 0.65

0.66211			
0.65947	0.65859		
0.65898	0.65881	0.65882	
0.65886	0.65882	0.65882	0.65882

$$= \frac{0.65}{2}\left[e^{-0.2^2} + 2e^{-0.85^2} + e^{-1.5^2}\right]$$

$$= 0.66211.$$

The next estimate uses $h = 0.65/2 = 0.325$:

$$\text{Integral} = \frac{h}{2}\left[f(a) + 2f(a+h) + 2f(a+2h) + 2f(a+3h) + f(b)\right]$$

$$= \frac{0.325}{2}\left[e^{-0.2^2} + 2e^{-0.525^2} + 2e^{-0.85^2} + 2e^{-1.175^2} + e^{-1.5^2}\right]$$

$$= 0.65947.$$

Observe that only two new function evaluations appear in the second estimate.
We now extrapolate:

$$\text{Improved} = 0.65947 + \frac{1}{3}[0.65947 - 0.66211]$$

$$= 0.65859.$$

Table 5.7 exhibits the calculations when we repeat the estimations, halving the h-value each time.

The Romberg Method for a Tabulated Function

We can apply the Romberg method to integrate a function known only as a table of evenly spaced function values, but now we cannot make h smaller. Instead, we use estimates of the integral with h doubled each time, just as we did to improve the estimates of derivatives in Section 5.1. Here is an example.

EXAMPLE 5.3 Use the Romberg method to get an improved estimate of the integral from $x = 1.8$ to $x = 3.4$ from the data in Table 5.6. In Example 5.1, we found an estimate of 23.9944 when $h = 0.2$. If we now use $h = 0.4$, we compute

$$\text{Integral} = (0.4/2)\,[6.050 + 2(9.025) + 2(13.464) + 2(20.086) + 29.964]$$

$$= 24.2328.$$

able of integrals over interval from 0.2 an initial h of 0.65

59		
81	0.65882	
82	0.65882	0.65882

$$= \frac{0.65}{2}[e^{-0.2^2} + 2e^{-0.85^2} + e^{-1.5^2}]$$

$$= 0.66211.$$

$h = 0.65/2 = 0.325$:

$$[f(a) + 2f(a+h) + 2f(a+2h) + 2f(a+3h) + f(b)]$$

$$\frac{.325}{2}[e^{-0.2^2} + 2e^{-0.525^2} + 2e^{-0.85^2} + 2e^{-1.175^2} + e^{-1.5^2}]$$

65947.

new function evaluations appear in the second estimate.

:

$$\text{proved} = 0.65947 + \frac{1}{3}[0.65947 - 0.66211]$$

$$= 0.65859.$$

calculations when we repeat the estimations, halving the h-value

ethod for a Tabulated Function

berg method to integrate a function known only as a table of evenly , but now we cannot make h smaller. Instead, we use estimates if bled each time, just as we did to improve the estimates of derivatives an example.

od to get an improved estimate of the integral from $x = 1.8$ to $x =$ able 5.6. In Example 5.1, we found an estimate of 23.9944 when $h = 0.4$, we compute

/2) [6.050 + 2(9.025) + 2(13.464) + 2(20.086) + 29.964]

328.

Table 5.8 Romberg table for Example 5.3

$h = 0.2$	23.9944	23.9149	23.9147
$h = 0.4$	24.2328	23.9181	
$h = 0.8$	25.1768		

We can extrapolate from these two estimates:

$$\text{Improved} = 23.9944 + (23.9944 - 24.2328)/3 = 23.9149.$$

Now, if we use $h = 0.8$, we get

$$\text{Integral} = (0.8/2)\,[6.050 + 2(13.464) + 29.964]$$
$$= 25.1768.$$

Using this with the estimate when $h = 0.4$:

$$\text{Improved} = 24.2328 + (24.2328 - 25.1768)/3$$
$$= 23.9181.$$

We can use these two improved estimates to extrapolate a second time:

$$\text{Further improved} = 23.9149 + (23.9149 - 23.9181)/15$$
$$= 23.9147.$$

Table 5.8 shows the results. Considering that the function values in Table 5.6 are given only to three decimals, this compares well to the analytical answer of 23.9144 and this is much better than the result from the single estimate with $h = 0.2$, which was 23.9944.

The Romberg method is applicable to a wide class of functions. Smoothness and continuity are not required. However, when $f(x)$ is discontinuous, we should make the evenly spaced points fall on the discontinuities. This can be done if we break the interval into subintervals that are bounded by the discontinuities.

An Algorithm for Romberg Integration

Given a function $f(x)$:

(Get user inputs).
Input
  a, b = endpoints of interval
  Maxstages = number of refinements

(Do the integration)

Set $h = (b - a)/2$.

(Do the lines of the table)
Set sum = $f(a) + 2 * f(a + h) + f(b)$.
Set integral(0, 0) = sum * $h/2$ (first value)
Set distance = 2 * h (distance between added points)
For stage = 1 To Maxstages Step 1 Do
    Set $h = h/2$.
    Set distance = distance/2.
    For i = 1 To 2^{stage} Step 1 Do
        Set $x = a - h + i$ * distance.
        Set sum = sum + 2 * $f(x)$.
    End Do (For i).
    Set integral(stage,0) = sum * $h/2$.
(Now extrapolate)
    For j = 1 To stage Step 1 Do
        Set integral(stage, j) = integral(stage, $j - 1$) +
            [integral(stage, $j - 1$) − integral(stage − 1, $j - 1$)]/($2^j - 1$)
    End Do (For j).
End Do (For stage)

The last computed value is the estimate of the integral.

An alternative stopping criterion is when two successive computations in a line differ by less than some tolerance value.

5.3 Simpson's Rules

The trapezoidal rule is based on approximating the function with a linear polynomial. We can fit the function better if we approximate it with a quadratic or a cubic interpolating polynomial. Simpson's rules are based on these approximations. There are two of these rules: *Simpson's 1/3 rule* and *Simpson's 3/8 rule*, so-named because the values 1/3 and 3/8 appear in their formulas.

We get the 1/3 rule by integrating the second-degree Newton–Gregory forward polynomial, which fits $f(x)$ at x-values of x_0, x_1, x_2, which are evenly spaced a distance h apart:

$$\begin{aligned}\int_{x_0}^{x_2} f(x)\,dx &\approx \int_{x_0}^{x_2}\left(f_0 + s\Delta f_0 + \frac{s(s-1)}{2}\Delta^2 f_0\right)dx \\ &= h\int_0^2\left(f_0 + s\Delta f_0 + \frac{s(s-1)}{2}\Delta^2 f_0\right)ds \\ &= hf_0 s\Big]_0^2 + h\Delta f_0\frac{s^2}{2}\Big]_0^2 + h\Delta^2 f_0\left(\frac{s^3}{6} - \frac{s^2}{4}\right)\Big]_0^2\end{aligned}$$

table)
2 * $f(a + h) + f(b)$.
sum * $h/2$ (first value)
h (distance between added points)
axstages Step 1 Do

istance/2.
ge Step 1 Do
+ i * distance.
n + 2 * $f(x)$.

,0) = sum * $h/2$.

e Step 1 Do
ge, j) = integral(stage, $j - 1$) +
ge, $j - 1$) − integral(stage − 1, $j - 1$)]/($2^j - 1$)

lue is the estimate of the integral.

ing criterion is when two successive computations in a line
ne tolerance value.

es

sed on approximating the function with a linear polynomial. We
r if we approximate it with a quadratic or a cubic interpolating
ules are based on these approximations. There are two of these
and *Simpson's 3/8 rule*, so-named because the values 1/3 and 3/8

integrating the second-degree Newton–Gregory forward polyno-
alues of x_0, x_1, x_2, which are evenly spaced a distance h apart:

$$= \int_{x_0}^{x_2} \left(f_0 + s\Delta f_0 + \frac{s(s-1)}{2} \Delta^2 f_0 \right) dx$$

$$h \int_0^2 \left(f_0 + s\Delta f_0 + \frac{s(s-1)}{2} \Delta^2 f_0 \right) ds$$

$$hf_0 s \Big]_0^2 + h\Delta f_0 \frac{s^2}{2} \Big]_0^2 + h\Delta^2 f_0 \left(\frac{s^3}{6} - \frac{s^2}{4} \right) \Big]_0^2$$

$$= h\left(2f_0 + 2\Delta f_0 + \frac{1}{3}\Delta^2 f_0\right) = \frac{h}{3}(f_0 + 4f_1 + f_2).*$$

We get the error by integrating the error of the polynomial:

$$\text{Error} = -\frac{1}{90} h^5 f^{(4)}(\xi), \qquad x_0 < \xi < x_2.$$

It is convenient to think of the strips defined by successive x-values as *panels*. For Simpson's 1/3 rule, there must be an even number of panels.

We get the 3/8 rule similarly, by integrating the third-degree Newton–Gregory interpolating polynomial that fits to four evenly spaced points, and its error term:

$$\int_{x_0}^{x_3} f(x)\,dx \approx \int_{x_0}^{x_3} P_3(x_s)\,dx = \frac{3h}{8}(f_0 + 3f_1 + 3f_2 + f_3).$$

$$\text{Error} = -\frac{3}{80} h^5 f^{(4)}(\xi_1), \qquad x_0 < \xi_1 < x_3.$$

If the number of panels is divisible by 3, the 3/8 rule applies. Observe that the error of the 3/8 rule is actually larger than for the 1/3 rule and both have a local error of $O(h^5)$. The global errors will be $O(h^4)$ for the same reason as with the trapezoidal rule.

You may wonder why we use the 3/8 rule when it has a larger error. One useful application of it is to find the integral from a table of values that has an odd number of panels. Still, the error should be less for a table with an odd number of points by applying the 3/8 rule for the first or last set of three panels and then using the 1/3 rule for the rest. Where the 3/8 rule is used, it is best to choose the panels at one end or the other, or at intermediate points where the function is most nearly straight.

In the example below, we compare the three rules. We will obtain the integral of $\exp(-x^2)$ between $x = 0.2$ and $x = 2.6$ with different values for h, the even spacing between points. This integral has no closed form; it is required to get values for the *error function,* a special function that is important in certain statistical applications and is related to another special function, the *gamma function.*

First, we will use MATLAB to get the true value of the integral:

```
EDU>> f = sym('exp(-x^2)')
  f =
     exp(-x^2)
EDU>> fint = int(f)
  fint =
     1/2*pi^(1/2)*erf(x)
EDU>> fintdef = int(f,.2,2.6)
  fintdef =
```

* This is the way that the rule is usually written and is responsible for its being called the 1/3 Rule. If the coefficient is written $2h/6$, it more closely parallels the trapezoidal rule and the 3/8 rule.

Table 5.9 Comparison of integration methods for the integral of $\exp(-x^2)$ between $x =$ 0.2 and 2.6

Number of panels	Trapezoidal rule Value	Trapezoidal rule Error	Simpson's 1/3 rule Value	Simpson's 1/3 rule Error	Simpson's 3/8 rule Value	Simpson's 3/8 rule Erorr
6	0.69378	−0.00513	0.68824	−0.00041	0.68723	−0.00142
12	0.68992	−0.00127	0.68863	−0.00002	0.68860	−0.00005
18	0.68921	−0.00056	0.68865	0.00000	0.68864	−0.00001
24	0.68897	−0.00031	0.68865	0.00000	0.68865	0.00000

```
    1/2*erf(13/5)*pi^(1/2) - 1/2*erf(1/5)*pi^(1/2)
EDU>> digits(10)
EDU>> vpa(fintdef)
  ans =
    .6886527145
```

In this, we define the function symbolically, ask for the indefinite integral (which does involve the error function), get the definite integral (but this is not numeric), and finally get the numeric answer with the vpa command.

EXAMPLE 5.4 Find the integral of $\exp(-x^2)$ between $x = 0.2$ and $x = 2.6$. Compare the results at varying values for h with the trapezoidal rule, Simpson's 1/3 rule, and Simpson's 3/8 rule.

Table 5.9 gives the results. With the trapezoidal method, five significant digits of accuracy are not obtained until almost 300 panels have been used. The 1/3 method is better than the 3/8, as we would expect. The ratio of errors when the h-value is halved is close to 2^4 for the 1/3 rule, not quite that for the 3/8 rule (we do not have enough data for a good value), and almost exactly 2^2 for the trapezoidal rule.

Formulas for Integration (Uniform spacing, $\Delta x = h$)

Trapezoidal rule:

$$\int_a^b f(x)\,dx = \frac{h}{2}(f_1 + 2f_2 + 2f_3 + \cdots + 2f_n + f_{n+1}) - \frac{(b-a)}{12}h^2 f''(\xi), \qquad a \le \xi \le b \tag{5.20}$$

ntegration methods for the integral of $\exp(-x^2)$ between $x =$

	Simpson's 1/3 rule		Simpson's 3/8 rule	
rror	Value	Error	Value	Erorr
00513	0.68824	−0.00041	0.68723	−0.00142
00127	0.68863	−0.00002	0.68860	−0.00005
00056	0.68865	0.00000	0.68864	−0.00001
00031	0.68865	0.00000	0.68865	0.00000

```
pi^(1/2) - 1/2*erf(1/5)*pi^(1/2)
```

ion symbolically, ask for the indefinite integral (which does
get the definite integral (but this is not numeric), and finally get
e vpa command.

^{2}) between $x = 0.2$ and $x = 2.6$. Compare the results at varying
oidal rule, Simpson's 1/3 rule, and Simpson's 3/8 rule.
ts. With the trapezoidal method, five significant digits of accu-
lmost 300 panels have been used. The 1/3 method is better than
. The ratio of errors when the h-value is halved is close to 2^4 for
for the 3/8 rule (we do not have enough data for a good value),
he trapezoidal rule.

(Uniform spacing, $\Delta x = h$)

$$2f_2 + 2f_3 + \cdots + 2f_n + f_{n+1})$$

$$-\frac{(b-a)}{12}h^2 f''(\xi), \qquad a \le \xi \le b \qquad (5.20)$$

Simpson's $\frac{1}{3}$ rule:

$$\int_a^b f(x)\,dx = \frac{h}{3}(f_1 + 4f_2 + 2f_3 + 4f_4 + 2f_5 + \cdots + 4f_n + f_{n+1})$$
$$- \frac{(b-a)}{180}h^4 f^{(4)}(\xi), \qquad a \le \xi \le b \qquad (5.21)$$

(requires an even number of panels)

Simpson's $\frac{3}{8}$ rule:

$$\int_a^b f(x)\,dx = \frac{3h}{8}(f_1 + 3f_2 + 3f_3 + 2f_4 + 3f_5 + 3f_6 + \cdots + 3f_n + f_{n+1})$$
$$- \frac{(b-a)}{80}h^4 f^{(4)}(\xi), \qquad a \le \xi \le b \qquad (5.22)$$

(requires a number of panels divisible by 3)

These formulas, based on approximating the integrand with a polynomial of different degree, are known as *Newton–Cotes formulas*.

It is of interest to see that each of these integration formulas is just the width of the interval, $(b - a)$, times an average value for the function within that interval. That average value is a sum of the weighted values divided by the sum of the weights. For example, if there are six panels (seven points),

Trapezoidal rule: Weights are [1 2 2 2 2 2 1], whose sum is 12 and $(b - a)/12 = h * (1/2)$.

Simpson's 1/3 rule: Weights are [1 4 2 4 2 4 1], whose sum is 18 and $(b - a)/18$ is $h * (1/3)$.

Simpson's 3/8 rule: Weights are [1 3 3 2 3 3 1], whose sum is 16 and $(b - a)/16$ is $h * (3/8)$.

Discontinuous Functions and Improper Integrals

If the function being integrated is discontinuous or whose slope is discontinuous, it is essential that the region be broken up into subintervals bounded by the discontinuities. (It could be that the chosen points within the interval fall at the points of discontinuity and that takes care of this.)

An improper integral is (a) one whose integrand becomes infinite at one or more points on the region of interest, or (b) one with infinity at one or both of the endpoints of the integration. Some improper integrals have a finite value; the integral is said to *converge*. If the limiting value of the integration as we approach the point of singularity is infinite, it is said to *diverge*. It is obvious that none of the integration rules that we have described will work which shows that the errors should be about proportional to h, precisely what Table 5.1 shows. In terms of the order relation, we see that error is $O(h)$. If we repeat this but begin with the Taylor series for $f(x - h)$, it turns out that

$$f'(x) = (f(x) - f(x - h))/h + f''(\zeta) * h/2, \tag{5.2}$$

where ζ is between x and $x - h$, so the two error terms are not identical though both are $O(h)$.

Now, if we add Eqs. (5.2) and (5.1), then divide by 2, we get the *central-difference approximation* to the derivative:

$$f'(x) = (f(x + h) - f(x - h))/(2h) - f'''(\xi)h^2/6. \tag{5.3}$$
$$\text{Error is } O(h^2).$$

We had to extend the two Taylor series by an additional term to get the error because the $f''(x)$ terms cancel.

This shows that using a central-difference approximation is a much preferred way to estimate the derivative; even though we use the same number of computations of the function at each step, we approach the answer much more rapidly. Table 5.2 illustrates this, showing that errors decrease about four fold when Δx is halved [as Eq. (5.3) predicts] and that a more accurate value is obtained.

All of this reminds us that it is best to center the x-value within the points used in the estimate, as we found for interpolation.

What we have found is also in accord with the *mean-value theorem for derivatives*:

$$\frac{f(b) - f(a)}{b - a} = f'(\xi), \quad \text{where } a < \xi < b.$$

The forward-difference approximation will give a value for $f'(x)$ at a point between x and $x + h$; the backward approximation gives a value at a point between $x - h$ and x; the central approximation at a point between $x - h$ and $x + h$. Unless the function behaves wildly near the point x, these three points are close to $x + h/2$, $x - h/2$, and x.

Table 5.2 Central-difference approximations for $f(x) = e^x \sin(x)$

Δx	Approximation	Error	Ratio of errors
0.05	4.15831	−0.00708	
0.05/2	4.16361	−0.00177	4.00
0.05/4	4.16496	−0.00042	4.21
0.05/8	4.16527	−0.00011	3.80
0.05/16	**4.16534**	**−0.00004**	**2.75**
0.05/32	4.16534	−0.00004	
0.05/64	4.16565	−0.00027	