

# Chapter 12

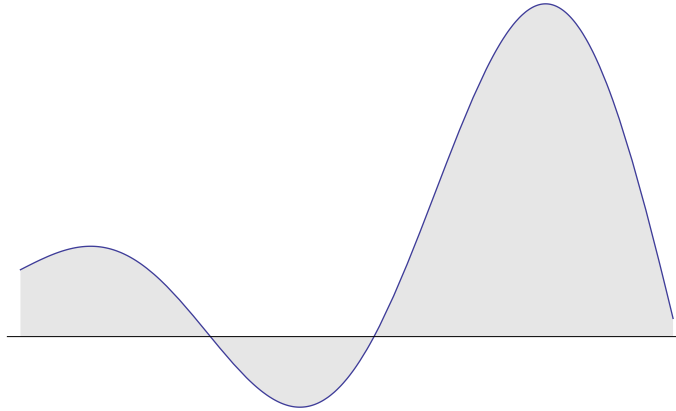
## Numerical Integration

Numerical differentiation methods compute approximations to the derivative of a function from known values of the function. Numerical integration uses the same information to compute numerical approximations to the integral of the function. An important use of both types of methods is estimation of derivatives and integrals for functions that are only known at isolated points, as is the case with for example measurement data. An important difference between differentiation and integration is that for most functions it is not possible to determine the integral via symbolic methods, but we can still compute numerical approximations to virtually any definite integral. Numerical integration methods are therefore more useful than numerical differentiation methods, and are essential in many practical situations.

We use the same general strategy for deriving numerical integration methods as we did for numerical differentiation methods: We find the polynomial that interpolates the function at some suitable points, and use the integral of the polynomial as an approximation to the function. This means that the truncation error can be analysed in basically the same way as for numerical differentiation. However, when it comes to round-off error, integration behaves differently from differentiation: Numerical integration is very *insensitive* to round-off errors, so we will ignore round-off in our analysis.

The mathematical definition of the integral is basically via a numerical integration method, and we therefore start by reviewing this definition. We then derive the simplest numerical integration method, and see how its error can be analysed. We then derive two other methods that are more accurate, but for these we just indicate how the error analysis can be done.

We emphasise that the general procedure for deriving both numerical dif-



**Figure 12.1.** The area under the graph of a function.

differentiation and integration methods with error analyses is the same with the exception that round-off errors are not of must interest for the integration methods.

### 12.1 General background on integration

Recall that if  $f(x)$  is a function, then the integral of  $f$  from  $x = a$  to  $x = b$  is written

$$\int_a^b f(x) dx.$$

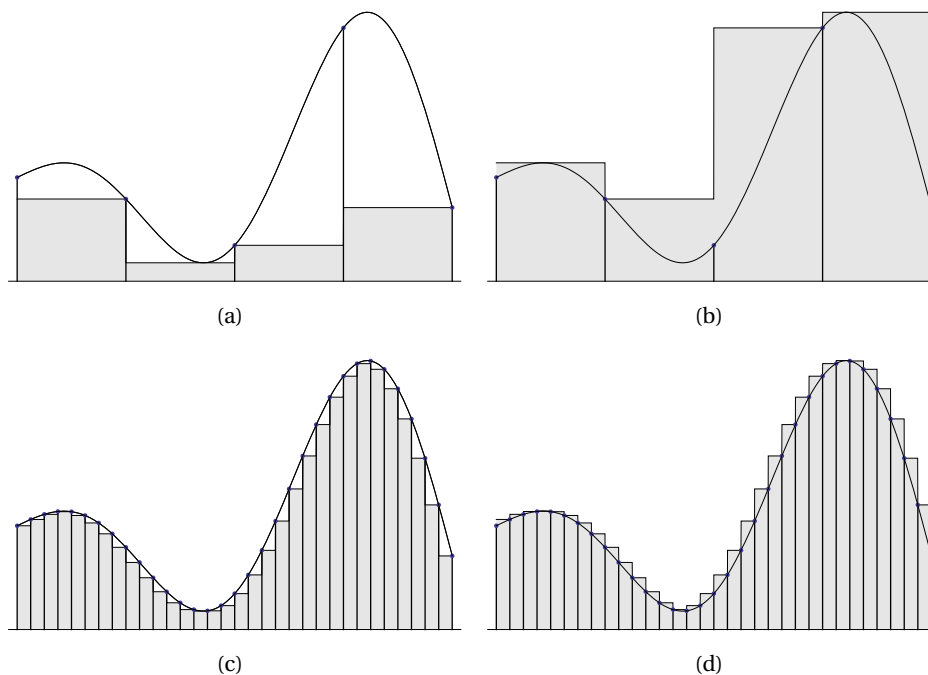
The integral gives the area under the graph of  $f$ , with the area under the positive part counting as positive area, and the area under the negative part of  $f$  counting as negative area, see figure 12.1.

Before we continue, we need to define a term which we will use repeatedly in our description of integration.

**Definition 12.1** (Partition). *Let  $a$  and  $b$  be two real numbers with  $a < b$ . A partition of  $[a, b]$  is a finite sequence  $\{x_i\}_{i=0}^n$  of increasing numbers in  $[a, b]$  with  $x_0 = a$  and  $x_n = b$ ,*

$$a = x_0 < x_1 < x_2 \cdots < x_{n-1} < x_n = b.$$

*The partition is said to be uniform if there is a fixed number  $h$ , called the step length, such that  $x_i - x_{i-1} = h = (b - a)/n$  for  $i = 1, \dots, n$ .*



**Figure 12.2.** The definition of the integral via inscribed and circumscribed step functions.

The traditional definition of the integral is based on a numerical approximation to the area. We pick a partition  $\{x_i\}_{i=0}^n$  of  $[a, b]$ , and in each subinterval  $[x_{i-1}, x_i]$  we determine the maximum and minimum of  $f$  (for convenience we assume that these values exist),

$$m_i = \min_{x \in [x_{i-1}, x_i]} f(x), \quad M_i = \max_{x \in [x_{i-1}, x_i]} f(x),$$

for  $i = 1, 2, \dots, n$ . We can then compute two obvious approximations to the integral by approximating  $f$  by two different functions which are both assumed to be constant on each interval  $[x_{i-1}, x_i]$ : The first has the constant value  $m_i$  and the other the value  $M_i$ . We then sum up the areas under each of the two step functions and end up with the two approximations

$$\underline{I} = \sum_{i=1}^n m_i(x_i - x_{i-1}), \quad \bar{I} = \sum_{i=1}^n M_i(x_i - x_{i-1}), \quad (12.1)$$

to the total area. In general, the first of these is too small, the other too large.

To define the integral, we consider larger partitions (smaller step lengths) and consider the limits of  $\underline{I}$  and  $\bar{I}$  as the distance between neighbouring  $x_i$ s goes

to zero. If those limits are the same, we say that  $f$  is integrable, and the integral is given by this limit.

**Definition 12.2** (Integral). Let  $f$  be a function defined on the interval  $[a, b]$ , and let  $\{x_i\}_{i=0}^n$  be a partition of  $[a, b]$ . Let  $m_i$  and  $M_i$  denote the minimum and maximum values of  $f$  over the interval  $[x_{i-1}, x_i]$ , respectively, assuming they exist. Consider the two numbers  $\underline{I}$  and  $\bar{I}$  defined in (12.1). If  $\sup \underline{I}$  and  $\inf \bar{I}$  both exist and are equal, where the sup and inf are taken over all possible partitions of  $[a, b]$ , the function  $f$  is said to be integrable, and the integral of  $f$  over  $[a, b]$  is defined by

$$I = \int_a^b f(x) dx = \sup \underline{I} = \inf \bar{I}.$$

This process is illustrated in figure 12.2 where we see how the piecewise constant approximations become better when the rectangles become narrower.

The above definition can be used as a numerical method for computing approximations to the integral. We choose to work with either maxima or minima, select a partition of  $[a, b]$  as in figure 12.2, and add together the areas of the rectangles. The problem with this technique is that it can be both difficult and time consuming to determine the maxima or minima, even on a computer. However, it can be shown that the integral has a property that is very useful when it comes to numerical computation.

**Theorem 12.3.** Suppose that  $f$  is integrable on the interval  $[a, b]$ , let  $\{x_i\}_{i=0}^n$  be a partition of  $[a, b]$ , and let  $t_i$  be a number in  $[x_{i-1}, x_i]$  for  $i = 1, \dots, n$ . Then the sum

$$\tilde{I} = \sum_{i=1}^n f(t_i)(x_i - x_{i-1}) \quad (12.2)$$

will converge to the integral when the distance between all neighbouring  $x_i$ s tends to zero.

Theorem 12.3 allows us to construct practical, numerical methods for computing the integral. We pick a partition of  $[a, b]$ , choose  $t_i$  equal to  $x_{i-1}$  or  $x_i$ , and compute the sum (12.2). It turns out that an even better choice is the more symmetric  $t_i = (x_i + x_{i-1})/2$  which leads to the approximation

$$I \approx \sum_{i=1}^n f((x_i + x_{i-1})/2)(x_i - x_{i-1}). \quad (12.3)$$

This is the so-called *midpoint rule* which we will study in the next section.

In general, we can derive numerical integration methods by splitting the interval  $[a, b]$  into small subintervals, approximate  $f$  by a polynomial on each subinterval, integrate this polynomial rather than  $f$ , and then add together the contributions from each subinterval. This is the strategy we will follow for deriving more advanced numerical integration methods, and this works as long as  $f$  can be approximated well by polynomials on each subinterval.

### Exercises

- 1 In this exercise we are going to study the definition of the integral for the function  $f(x) = e^x$  on the interval  $[0, 1]$ .
  - a) Determine lower and upper sums for a uniform partition consisting of 10 subintervals.
  - b) Determine the absolute and relative errors of the sums in (a) compared to the exact value  $e - 1 = 1.718281828$  of the integral.
  - c) Write a program for calculating the lower and upper sums in this example. How many subintervals are needed to achieve an absolute error less than  $3 \times 10^{-3}$ ?

## 12.2 The midpoint rule for numerical integration

We have already introduced the midpoint rule (12.3) for numerical integration. In our standard framework for numerical methods based on polynomial approximation, we can consider this as using a constant approximation to the function  $f$  on each subinterval. Note that in the following we will always assume the partition to be uniform.

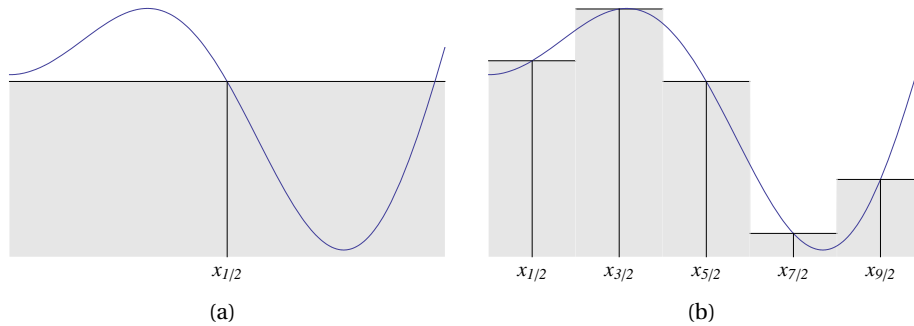
**Algorithm 12.4.** Let  $f$  be a function which is integrable on the interval  $[a, b]$ , and let  $\{x_i\}_{i=0}^n$  be a uniform partition of  $[a, b]$ . In the midpoint rule, the integral of  $f$  is approximated by

$$\int_a^b f(x) dx \approx I_{\text{mid}}(h) = h \sum_{i=1}^n f(x_{i-1/2}), \quad (12.4)$$

where

$$x_{i-1/2} = (x_{i-1} + x_i)/2 = a + (i - 1/2)h.$$

This may seem like a strangely formulated algorithm, but all there is to do is to compute the sum on the right in (12.4). The method is illustrated in figure 12.3 in the cases where we have 1 and 5 subintervals.



**Figure 12.3.** The midpoint rule with one subinterval (a) and five subintervals (b).

### 12.2.1 A detailed algorithm

Algorithm 12.4 describes the midpoint rule, but lacks a lot of detail. In this section we give a more detailed algorithm.

Whenever we compute a quantity numerically, we should try and estimate the error, otherwise we have no idea of the quality of our computation. We did this when we discussed algorithms for finding roots of equations in chapter 10, and we can do exactly the same here: We compute the integral for decreasing step lengths, and stop the computations when the difference between two successive approximations is less than the tolerance. More precisely, we choose an initial step length  $h_0$  and compute the approximations

$$I_{\text{mid}}(h_0), I_{\text{mid}}(h_1), \dots, I_{\text{mid}}(h_k), \dots,$$

where  $h_k = h_0/2^k$ . Suppose  $I_{\text{mid}}(h_k)$  is our latest approximation. Then we estimate the relative error by the number

$$\frac{|I_{\text{mid}}(h_k) - I_{\text{mid}}(h_{k-1})|}{|I_{\text{mid}}(h_k)|},$$

and stop the computations if this is smaller than  $\epsilon$ . To avoid potential division by zero, we use the test

$$|I_{\text{mid}}(h_k) - I_{\text{mid}}(h_{k-1})| \leq \epsilon |I_{\text{mid}}(h_k)|.$$

As always, we should also limit the number of approximations that are computed, so we count the number of times we divide the subintervals, and stop when we reach a predefined limit which we call  $M$ .

**Algorithm 12.5.** Suppose the function  $f$ , the interval  $[a, b]$ , the length  $n_0$  of the initial partition, a positive tolerance  $\epsilon < 1$ , and the maximum number of iterations  $M$  are given. The following algorithm will compute a sequence of approximations to  $\int_a^b f(x) dx$  by the midpoint rule, until the estimated relative error is smaller than  $\epsilon$ , or the maximum number of computed approximations reach  $M$ . The final approximation is stored in  $I$ .

```

 $n := n_0; \quad h := (b - a) / n;$ 
 $I := 0; \quad x := a + h/2;$ 
for  $k := 1, 2, \dots, n$ 
     $I := I + f(x);$ 
     $x := x + h;$ 
 $j := 1;$ 
 $I := h * I;$ 
 $abserr := |I|;$ 
while  $j < M$  and  $abserr > \epsilon * |I|$ 
     $j := j + 1;$ 
     $Ip := I;$ 
     $n := 2n; \quad h := (b - a) / n;$ 
     $I := 0; \quad x := a + h/2;$ 
    for  $k := 1, 2, \dots, n$ 
         $I := I + f(x);$ 
         $x := x + h;$ 
     $I := h * I;$ 
     $abserr := |I - Ip|;$ 

```

Note that we compute the first approximation outside the main loop. This is necessary in order to have meaningful estimates of the relative error the first two times we reach the while loop (the first time we reach the while loop we will always get past the condition). We store the previous approximation in  $Ip$  and use this to estimate the error in the next iteration.

In the coming sections we will describe two other methods for numerical integration. These can be implemented in algorithms similar to Algorithm 12.5. In fact, the only difference will be how the actual approximation to the integral is computed.

**Example 12.6.** Let us try the midpoint rule on an example. As usual, it is wise to test on an example where we know the answer, so we can easily check the quality

of the method. We choose the integral

$$\int_0^1 \cos x \, dx = \sin 1 \approx 0.8414709848$$

where the exact answer is easy to compute by traditional, symbolic methods. To test the method, we split the interval into  $2^k$  subintervals, for  $k = 1, 2, \dots, 10$ , i.e., we halve the step length each time. The result is

$h$	$I_{\text{mid}}(h)$	Error
0.500000	0.85030065	$-8.8 \times 10^{-3}$
0.250000	0.84366632	$-2.2 \times 10^{-3}$
0.125000	0.84201907	$-5.5 \times 10^{-4}$
0.062500	0.84160796	$-1.4 \times 10^{-4}$
0.031250	0.84150523	$-3.4 \times 10^{-5}$
0.015625	0.84147954	$-8.6 \times 10^{-6}$
0.007813	0.84147312	$-2.1 \times 10^{-6}$
0.003906	0.84147152	$-5.3 \times 10^{-7}$
0.001953	0.84147112	$-1.3 \times 10^{-7}$
0.000977	0.84147102	$-3.3 \times 10^{-8}$

By error, we here mean

$$\int_0^1 f(x) \, dx - I_{\text{mid}}(h).$$

Note that each time the step length is halved, the error seems to be reduced by a factor of 4. ■

### 12.2.2 The error

Algorithm 12.5 determines a numerical approximation to the integral, and even estimates the error. However, we must remember that the error that is computed is not always reliable, so we should try and understand the error better. We do this in two steps. First we analyse the error in the situation where we use a very simple partition with only one subinterval, the so-called *local error*. Then we use this result to obtain an estimate of the error in the general case — this is often referred to as the *global error*.

#### Local error analysis

Suppose we use the midpoint rule with just one subinterval. We want to study the error

$$\int_a^b f(x) \, dx - f(a_{1/2})(b - a), \quad a_{1/2} = (a + b)/2. \quad (12.5)$$



Once again, a Taylor polynomial with remainder helps us out. We expand  $f(x)$  about the midpoint  $a_{1/2}$  and obtain,

$$f(x) = f(a_{1/2}) + (x - a_{1/2})f'(a_{1/2}) + \frac{(x - a_{1/2})^2}{2}f''(\xi),$$

where  $\xi$  is a number in the interval  $(a_{1/2}, x)$  that depends on  $x$ . Next, we integrate the Taylor expansion and obtain

$$\begin{aligned} \int_a^b f(x) dx &= \int_a^b \left( f(a_{1/2}) + (x - a_{1/2})f'(a_{1/2}) + \frac{(x - a_{1/2})^2}{2}f''(\xi) \right) dx \\ &= f(a_{1/2})(b - a) + \frac{f'(a_{1/2})}{2} [(x - a_{1/2})^2]_a^b + \frac{1}{2} \int_a^b (x - a_{1/2})^2 f''(\xi) dx \\ &= f(a_{1/2})(b - a) + \frac{1}{2} \int_a^b (x - a_{1/2})^2 f''(\xi) dx, \end{aligned} \tag{12.6}$$

since the middle term is zero. This leads to an expression for the error,

$$\left| \int_a^b f(x) dx - f(a_{1/2})(b - a) \right| = \frac{1}{2} \left| \int_a^b (x - a_{1/2})^2 f''(\xi) dx \right|. \tag{12.7}$$

Let us simplify the right-hand side of this expression and explain afterwards. We have

$$\begin{aligned} \frac{1}{2} \left| \int_a^b (x - a_{1/2})^2 f''(\xi) dx \right| &\leq \frac{1}{2} \int_a^b |(x - a_{1/2})^2 f''(\xi)| dx \\ &= \frac{1}{2} \int_a^b (x - a_{1/2})^2 |f''(\xi)| dx \\ &\leq \frac{M}{2} \int_a^b (x - a_{1/2})^2 dx \\ &= \frac{M}{2} \frac{1}{3} [(x - a_{1/2})^3]_a^b \\ &= \frac{M}{6} ((b - a_{1/2})^3 - (a - a_{1/2})^3) \\ &= \frac{M}{24} (b - a)^3, \end{aligned} \tag{12.8}$$

where  $M = \max_{x \in [a, b]} |f''(x)|$ . The first inequality is valid because when we move the absolute value sign inside the integral sign, the function that we integrate becomes nonnegative everywhere. This means that in the areas where the integrand in the original expression is negative, everything is now positive, and hence the second integral is larger than the first.

Next there is an equality which is valid because  $(x - a_{1/2})^2$  is never negative. The next inequality follows because we replace  $|f''(\xi)|$  with its maximum on the

interval  $[a, b]$ . The next step is just the evaluation of the integral of  $(x - a_{1/2})^2$ , and the last equality follows since  $(b - a_{1/2})^3 = -(a - a_{1/2})^3 = (b - a)^3/8$ . This proves the following lemma.

**Lemma 12.7.** *Let  $f$  be a continuous function whose first two derivatives are continuous on the interval  $[a, b]$ . The error in the midpoint rule, with only one interval, is bounded by*

$$\left| \int_a^b f(x) dx - f(a_{1/2})(b - a) \right| \leq \frac{M}{24}(b - a)^3,$$

where  $M = \max_{x \in [a, b]} |f''(x)|$  and  $a_{1/2} = (a + b)/2$ .

Before we continue, let us sum up the procedure that led up to lemma 12.7 without focusing on the details: Start with the error (12.5) and replace  $f(x)$  by its linear Taylor polynomial with remainder. When we integrate the Taylor polynomial, the linear term becomes zero, and we are left with (12.7). At this point we use some standard techniques that give us the final inequality.

The importance of lemma 12.7 lies in the factor  $(b - a)^3$ . This means that if we reduce the size of the interval to half its width, the error in the midpoint rule will be reduced by a factor of 8.

### Global error analysis

Above, we analysed the error on one subinterval. Now we want to see what happens when we add together the contributions from many subintervals.

We consider the general case where we have a partition that divides  $[a, b]$  into  $n$  subintervals, each of width  $h$ . On each subinterval we use the simple midpoint rule that we just analysed,

$$I = \int_a^b f(x) dx = \sum_{i=1}^n \int_{x_{i-1}}^{x_i} f(x) dx \approx \sum_{i=1}^n f(x_{i-1/2})h.$$

The total error is then

$$I - I_{\text{mid}} = \sum_{i=1}^n \left( \int_{x_{i-1}}^{x_i} f(x) dx - f(x_{i-1/2})h \right).$$

We note that the expression inside the parenthesis is just the local error on the

interval  $[x_{i-1}, x_i]$ . We therefore have

$$\begin{aligned} |I - I_{\text{mid}}| &= \left| \sum_{i=1}^n \left( \int_{x_{i-1}}^{x_i} f(x) dx - f(x_{i-1/2})h \right) \right| \\ &\leq \sum_{i=1}^n \left| \int_{x_{i-1}}^{x_i} f(x) dx - f(x_{i-1/2})h \right| \\ &\leq \sum_{i=1}^n \frac{h^3}{24} M_i \end{aligned} \quad (12.9)$$

where  $M_i$  is the maximum of  $|f''(x)|$  on the interval  $[x_{i-1}, x_i]$ . The first of these inequalities is just the triangle inequality, while the second inequality follows from lemma 12.7. To simplify the expression (12.9), we extend the maximum on  $[x_{i-1}, x_i]$  to all of  $[a, b]$ . This cannot make the maximum smaller, so for all  $i$  we have

$$M_i = \max_{x \in [x_{i-1}, x_i]} |f''(x)| \leq \max_{x \in [a, b]} |f''(x)| = M.$$

Now we can simplify (12.9) further,

$$\sum_{i=1}^n \frac{h^3}{24} M_i \leq \sum_{i=1}^n \frac{h^3}{24} M = \frac{h^3}{24} nM. \quad (12.10)$$

Here, we need one final little observation. Recall that  $h = (b-a)/n$ , so  $hn = b-a$ . If we insert this in (12.10), we obtain our main error estimate.

**Theorem 12.8.** *Suppose that  $f$  and its first two derivatives are continuous on the interval  $[a, b]$ , and that the integral of  $f$  on  $[a, b]$  is approximated by the midpoint rule with  $n$  subintervals of equal width,*

$$I = \int_a^b f(x) dx \approx I_{\text{mid}} = \sum_{i=1}^n f(x_{i-1/2})h.$$

*Then the error is bounded by*

$$|I - I_{\text{mid}}| \leq (b-a) \frac{h^2}{24} \max_{x \in [a, b]} |f''(x)|, \quad (12.11)$$

*where  $x_{i-1/2} = a + (i-1/2)h$ .*

This confirms the error behaviour that we saw in example 12.6: If  $h$  is reduced by a factor of 2, the error is reduced by a factor of  $2^2 = 4$ .

One notable omission in our discussion of the error in the midpoint rule is round-off error, which was a major concern in our study of numerical differentiation. The good news is that round-off error is not usually a problem in numerical integration. The only situation where round-off may cause problems is when the value of the integral is 0. In such a situation we may potentially add many numbers that sum to 0, and this may lead to cancellation effects. However, this is so rare that we will not discuss it here.

### 12.2.3 Estimating the step length

The error estimate (12.11) lets us play a standard game: If someone demands that we compute an integral with error smaller than  $\epsilon$ , we can find a step length  $h$  that guarantees that we meet this demand. To make sure that the error is smaller than  $\epsilon$ , we enforce the inequality

$$(b-a) \frac{h^2}{24} \max_{x \in [a,b]} |f''(x)| \leq \epsilon$$

which we can easily solve for  $h$ ,

$$h \leq \sqrt{\frac{24\epsilon}{(b-a)M}}, \quad M = \max_{x \in [a,b]} |f''(x)|.$$

This is not quite as simple as it may look since we will have to estimate  $M$ , the maximum value of the second derivative, over the whole interval of integration  $[a, b]$ . This can be difficult, but in some cases it is certainly possible, see exercise 3.

### Exercises

- 1 Calculate an approximation to the integral

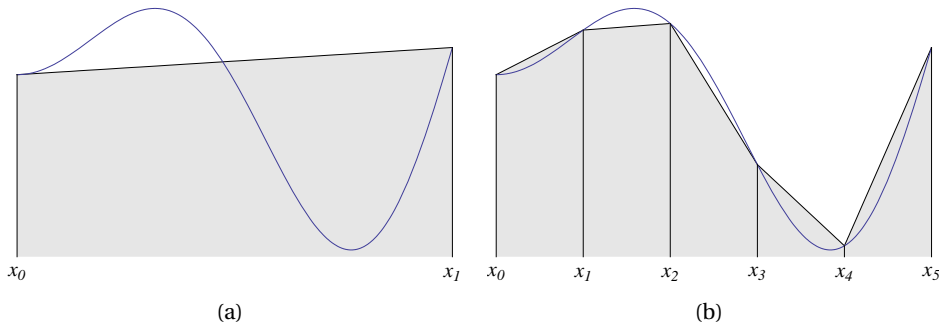
$$\int_0^{\pi/2} \frac{\sin x}{1+x^2} dx = 0.526978557614\dots$$

with the midpoint rule. Split the interval into 6 subintervals.

- 2 In this exercise you are going to program algorithm 12.5. If you cannot program, use the midpoint algorithm with 10 subintervals, check the error, and skip (b).

- a) Write a program that implements the midpoint rule as in algorithm 12.5 and test it on the integral

$$\int_0^1 e^x dx = e - 1.$$



**Figure 12.4.** The trapezoidal rule with one subinterval (a) and five subintervals (b).

- b) Determine a value of  $h$  that guarantees that the absolute error is smaller than  $10^{-10}$ . Run your program and check what the actual error is for this value of  $h$ . (You may have to adjust algorithm 12.5 slightly and print the absolute error.)

- 3 Repeat the previous exercise, but compute the integral

$$\int_2^6 \ln x \, dx = \ln(11664) - 4.$$

- 4 Redo the local error analysis for the midpoint rule, but replace both  $f(x)$  and  $f(a_{1/2})$  by linear Taylor polynomials with remainders about the left end point  $a$ . What happens to the error estimate?

### 12.3 The trapezoidal rule

The midpoint rule is based on a very simple polynomial approximation to the function  $f$  to be integrated on each subinterval; we simply use a constant approximation that interpolates the function value at the middle point. We are now going to consider a natural alternative; we approximate  $f$  on each subinterval with the secant that interpolates  $f$  at both ends of the subinterval.

The situation is shown in figure 12.4a. The approximation to the integral is the area of the trapezoidal polygon under the secant so we have

$$\int_a^b f(x) \, dx \approx \frac{f(a) + f(b)}{2} (b - a). \quad (12.12)$$

To get good accuracy, we will have to split  $[a, b]$  into subintervals with a partition and use the trapezoidal approximation on each subinterval, as in figure 12.4b. If we have a uniform partition  $\{x_i\}_{i=0}^n$  with step length  $h$ , we get the approximation

$$\int_a^b f(x) \, dx = \sum_{i=1}^n \int_{x_{i-1}}^{x_i} f(x) \, dx \approx \sum_{i=1}^n \frac{f(x_{i-1}) + f(x_i)}{2} h. \quad (12.13)$$

We should always aim to make our computational methods as efficient as possible, and in this case an improvement is possible. Note that on the interval  $[x_{i-1}, x_i]$  we use the function values  $f(x_{i-1})$  and  $f(x_i)$ , and on the next interval we use the values  $f(x_i)$  and  $f(x_{i+1})$ . All function values, except the first and last, therefore occur twice in the sum on the right in (12.13). This means that if we implement this formula directly we do a lot of unnecessary work. From this the following observation follows.

**Observation 12.9** (Trapezoidal rule). *Suppose we have a function  $f$  defined on an interval  $[a, b]$  and a partition  $\{x_i\}_{i=0}^n$  of  $[a, b]$ . If we approximate  $f$  by its secant on each subinterval and approximate the integral of  $f$  by the integral of the resulting piecewise linear approximation, we obtain the approximation*

$$\int_a^b f(x) dx \approx I_{\text{trap}}(h) = h \left( \frac{f(a) + f(b)}{2} + \sum_{i=1}^{n-1} f(x_i) \right). \quad (12.14)$$

Once we have the formula (12.14), we can easily derive an algorithm similar to algorithm 12.5. In fact the two algorithms are identical except for the part that calculates the approximations to the integral, so we will not discuss this further.

**Example 12.10.** We test the trapezoidal rule on the same example as the midpoint rule,

$$\int_0^1 \cos x dx = \sin 1 \approx 0.8414709848.$$

As in example 12.6 we split the interval into  $2^k$  subintervals, for  $k = 1, 2, \dots, 10$ . The resulting approximations are

$h$	$I_{\text{trap}}(h)$	Error
0.500000	0.82386686	$1.8 \times 10^{-2}$
0.250000	0.83708375	$4.4 \times 10^{-3}$
0.125000	0.84037503	$1.1 \times 10^{-3}$
0.062500	0.84119705	$2.7 \times 10^{-4}$
0.031250	0.84140250	$6.8 \times 10^{-5}$
0.015625	0.84145386	$1.7 \times 10^{-5}$
0.007813	0.84146670	$4.3 \times 10^{-6}$
0.003906	0.84146991	$1.1 \times 10^{-6}$
0.001953	0.84147072	$2.7 \times 10^{-7}$
0.000977	0.84147092	$6.7 \times 10^{-8}$

where the error is defined by

$$\int_0^1 f(x) dx - I_{\text{trap}}(h).$$

We note that each time the step length is halved, the error is reduced by a factor of 4, just as for the midpoint rule. But we also note that even though we now use two function values in each subinterval to estimate the integral, the error is actually twice as big as it was for the midpoint rule. ■

### 12.3.1 The error

Our next step is to analyse the error in the trapezoidal rule. We follow the same strategy as for the midpoint rule and use Taylor polynomials. Because of the similarities with the midpoint rule, we skip some of the details.

#### The local error

We first study the error in the approximation (12.12) where we only have one secant. In this case the error is given by

$$\left| \int_a^b f(x) dx - \frac{f(a) + f(b)}{2} (b - a) \right|, \quad (12.15)$$

and the first step is to expand the function values  $f(x)$ ,  $f(a)$ , and  $f(b)$  in Taylor series about the midpoint  $a_{1/2}$ ,

$$\begin{aligned} f(x) &= f(a_{1/2}) + (x - a_{1/2})f'(a_{1/2}) + \frac{(x - a_{1/2})^2}{2} f''(\xi_1), \\ f(a) &= f(a_{1/2}) + (a - a_{1/2})f'(a_{1/2}) + \frac{(a - a_{1/2})^2}{2} f''(\xi_2), \\ f(b) &= f(a_{1/2}) + (b - a_{1/2})f'(a_{1/2}) + \frac{(b - a_{1/2})^2}{2} f''(\xi_3), \end{aligned}$$

where  $\xi_1 \in (a_{1/2}, x)$ ,  $\xi_2 \in (a, a_{1/2})$ , and  $\xi_3 \in (a_{1/2}, b)$ . The integration of the Taylor series for  $f(x)$  we did in (12.6) so we just quote the result here,

$$\int_a^b f(x) dx = f(a_{1/2})(b - a) + \frac{1}{2} \int_a^b (x - a_{1/2})^2 f''(\xi_1) dx. \quad (12.16)$$

We note that  $a - a_{1/2} = -(b - a)/2$  and  $b - a_{1/2} = (b - a)/2$ , so the sum of the Taylor series for  $f(a)$  and  $f(b)$  is

$$f(a) + f(b) = 2f(a_{1/2}) + \frac{(b - a)^2}{8} f''(\xi_2) + \frac{(b - a)^2}{8} f''(\xi_3). \quad (12.17)$$

If we insert (12.16) and (12.17) in the expression for the error (12.15), the first two terms cancel, and we obtain

$$\begin{aligned} & \left| \int_a^b f(x) dx - \frac{f(a) + f(b)}{2} (b - a) \right| \\ &= \left| \frac{1}{2} \int_a^b (x - a_{1/2})^2 f''(\xi_1) dx - \frac{(b-a)^3}{16} f''(\xi_2) - \frac{(b-a)^3}{16} f''(\xi_3) \right| \\ &\leq \left| \frac{1}{2} \int_a^b (x - a_{1/2})^2 f''(\xi_1) dx \right| + \frac{(b-a)^3}{16} |f''(\xi_2)| + \frac{(b-a)^3}{16} |f''(\xi_3)|. \end{aligned}$$

The last relation is just an application of the triangle inequality. The first term we estimated in (12.8), and in the last two we use the standard trick and take maximum values of  $|f''(x)|$  over all of  $[a, b]$ . Then we end up with

$$\begin{aligned} \left| \int_a^b f(x) dx - \frac{f(a) + f(b)}{2} (b - a) \right| &\leq \frac{M}{24} (b - a)^3 + \frac{M}{16} (b - a)^3 + \frac{M}{16} (b - a)^3 \\ &= \frac{M}{6} (b - a)^3. \end{aligned}$$

Let us sum this up in a lemma.

**Lemma 12.11.** *Let  $f$  be a continuous function whose first two derivatives are continuous on the interval  $[a, b]$ . The error in the trapezoidal rule, with only one secant based at  $a$  and  $b$ , is bounded by*

$$\left| \int_a^b f(x) dx - \frac{f(a) + f(b)}{2} (b - a) \right| \leq \frac{M}{6} (b - a)^3,$$

where  $M = \max_{x \in [a, b]} |f''(x)|$ .

This lemma is completely analogous to lemma 12.7 which describes the local error in the midpoint rule. We particularly notice that even though the trapezoidal rule uses two values of  $f$ , the error estimate is slightly larger than the estimate for the midpoint rule. The most important feature is the exponent on  $(b - a)$ , which tells us how quickly the error goes to 0 when the interval width is reduced, and from this point of view the two methods are the same. In other words, we have gained nothing by approximating  $f$  by a linear function instead of a constant. This does not mean that the trapezoidal rule is bad, it rather means that the midpoint rule is surprisingly good.



### Global error

We can find an expression for the global error in the trapezoidal rule in exactly the same way as we did for the midpoint rule, so we skip the proof.

**Theorem 12.12.** *Suppose that  $f$  and its first two derivatives are continuous on the interval  $[a, b]$ , and that the integral of  $f$  on  $[a, b]$  is approximated by the trapezoidal rule with  $n$  subintervals of equal width  $h$ ,*

$$I = \int_a^b f(x) dx \approx I_{\text{trap}} = h \left( \frac{f(a) + f(b)}{2} + \sum_{i=1}^{n-1} f(x_i) \right).$$

*Then the error is bounded by*

$$|I - I_{\text{trap}}| \leq (b - a) \frac{h^2}{6} \max_{x \in [a, b]} |f''(x)|. \quad (12.18)$$

The error estimate for the trapezoidal rule is not best possible in the sense that it is possible to derive a better error estimate (using other techniques) with the smaller constant  $1/12$  instead of  $1/6$ . However, the fact remains that the trapezoidal rule is a bit disappointing compared to the midpoint rule, just as we saw in example 12.10.

### Exercises

- 1 Calculate an approximation to the integral

$$\int_0^{\pi/2} \frac{\sin x}{1+x^2} dx = 0.526978557614\dots$$

with the trapezoidal rule. Split the interval into 6 subintervals.

- 2 In this exercise you are going to program an algorithm like algorithm 12.5 for the trapezoidal rule. If you cannot program, use the trapezoidal rule manually with 10 subintervals, check the error, and skip the second part of (b).

- a) Write a program that implements the midpoint rule as in algorithm 12.5 and test it on the integral

$$\int_0^1 e^x dx = e - 1.$$

- b) Determine a value of  $h$  that guarantees that the absolute error is smaller than  $10^{-10}$ . Run your program and check what the actual error is for this value of  $h$ . (You may have to adjust algorithm 12.5 slightly and print the absolute error.)

- 3 Fill in the details in the derivation of lemma 12.11 from (12.16) and (12.17).
- 4 In this exercise we are going to do an alternative error analysis for the trapezoidal rule. Use the same procedure as in section 12.3.1, but expand both the function values  $f(x)$  and  $f(b)$  in Taylor series about  $a$ . Compare the resulting error estimate with lemma 12.11.
- 5 When  $h$  is halved in the trapezoidal rule, some of the function values used with step length  $h/2$  are the same as those used for step length  $h$ . Derive a formula for the trapezoidal rule with step length  $h/2$  that makes it easy to avoid recomputing the function values that were computed on the previous level.

## 12.4 Simpson's rule

The final method for numerical integration that we consider is *Simpson's rule*. This method is based on approximating  $f$  by a parabola on each subinterval, which makes the derivation a bit more involved. The error analysis is essentially the same as before, but because the expressions are more complicated, we omit it here.

### 12.4.1 Derivation of Simpson's rule

As for the other methods, we derive Simpson's rule in the simplest case where we approximate  $f$  by one parabola on the whole interval  $[a, b]$ . We find the polynomial  $p_2$  that interpolates  $f$  at  $a$ ,  $a_{1/2} = (a + b)/2$  and  $b$ , and approximate the integral of  $f$  by the integral of  $p_2$ . We could find  $p_2$  via the Newton form, but in this case it is easier to use the Lagrange form. Another simplification is to first construct Simpson's rule in the case where  $a = -1$ ,  $a_{1/2} = 0$ , and  $b = 1$ , and then generalise afterwards.

#### Simpson's rule on $[-1, 1]$

The Lagrange form of the polynomial that interpolates  $f$  at  $-1$ ,  $0$ , and  $1$  is given by

$$p_2(x) = f(-1) \frac{x(x-1)}{2} - f(0)(x+1)(x-1) + f(1) \frac{(x+1)x}{2},$$

and it is easy to check that the interpolation conditions hold. To integrate  $p_2$ , we must integrate each of the three polynomials in this expression. For the first one we have

$$\frac{1}{2} \int_{-1}^1 x(x-1) dx = \frac{1}{2} \int_{-1}^1 (x^2 - x) dx = \frac{1}{2} \left[ \frac{1}{3}x^3 - \frac{1}{2}x^2 \right]_{-1}^1 = \frac{1}{3}.$$

Similarly, we find

$$-\int_{-1}^1 (x+1)(x-1) dx = \frac{4}{3}, \quad \frac{1}{2} \int_{-1}^1 (x+1)x dx = \frac{1}{3}.$$

On the interval  $[-1, 1]$ , Simpson's rule therefore corresponds to the approximation

$$\int_{-1}^1 f(x) dx \approx \frac{1}{3}(f(-1) + 4f(0) + f(1)). \quad (12.19)$$

**Simpson's rule on  $[a, b]$**

To obtain an approximation of the integral on the interval  $[a, b]$ , we use a standard technique. Suppose that  $x$  and  $y$  are related by

$$x = (b - a)\frac{y + 1}{2} + a \quad (12.20)$$

so that when  $y$  varies in the interval  $[-1, 1]$ , then  $x$  will vary in the interval  $[a, b]$ . We are going to use the relation (12.20) as a substitution in an integral, so we note that  $dx = (b - a)dy/2$ . We therefore have

$$\int_a^b f(x) dx = \frac{b - a}{2} \int_{-1}^1 f\left(\frac{b - a}{2}(y + 1) + a\right) dy = \frac{b - a}{2} \int_{-1}^1 \tilde{f}(y) dy, \quad (12.21)$$

where

$$\tilde{f}(y) = f\left(\frac{b - a}{2}(y + 1) + a\right).$$

To determine an approximation to the integral of  $\tilde{f}$  on the interval  $[-1, 1]$ , we use Simpson's rule (12.19). The result is

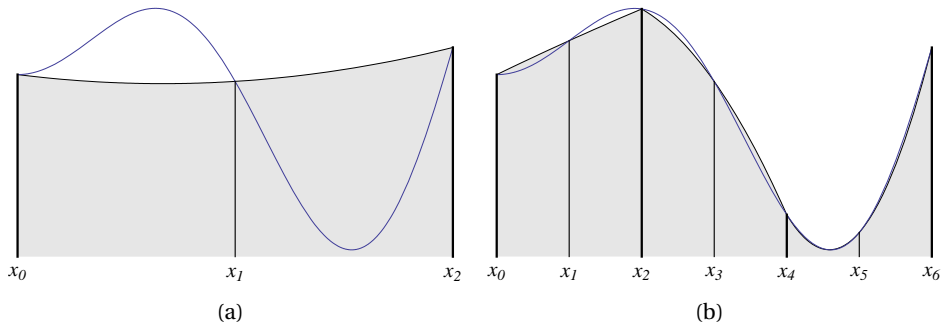
$$\int_{-1}^1 \tilde{f}(y) dy \approx \frac{1}{3}(\tilde{f}(-1) + 4\tilde{f}(0) + \tilde{f}(1)) = \frac{1}{3}(f(a) + 4f(a_{1/2}) + f(b)),$$

since the relation in (12.20) maps  $-1$  to  $a$ , the midpoint  $0$  to  $a_{1/2} = (a + b)/2$ , and the right endpoint  $b$  to  $1$ . If we insert this in (12.21), we obtain Simpson's rule for the general interval  $[a, b]$ , see figure 12.5a.

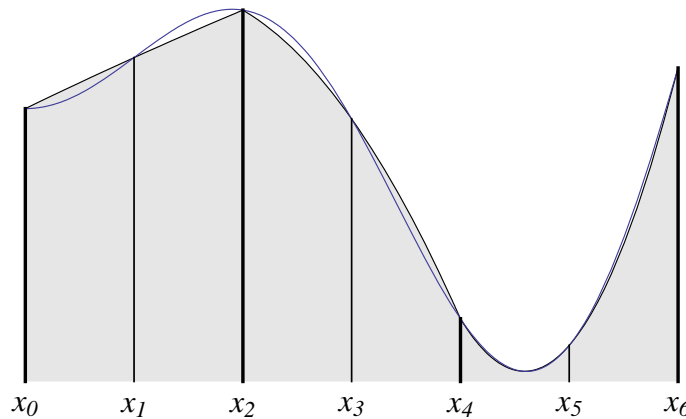
**Observation 12.13.** *Let  $f$  be an integrable function on the interval  $[a, b]$ . If  $f$  is interpolated by a quadratic polynomial  $p_2$  at the points  $a$ ,  $a_{1/2} = (a + b)/2$  and  $b$ , then the integral of  $f$  can be approximated by the integral of  $p_2$ ,*

$$\int_a^b f(x) dx \approx \int_a^b p_2(x) dx = \frac{b - a}{6}(f(a) + 4f(a_{1/2}) + f(b)). \quad (12.22)$$

We may just as well derive this formula by doing the interpolation directly on the interval  $[a, b]$ , but then the algebra becomes quite messy.



**Figure 12.5.** Simpson's rule with one subinterval (a) and three subintervals (b).



**Figure 12.6.** Simpson's rule with three subintervals.

### 12.4.2 Composite Simpson's rule

In practice, we will usually divide the interval  $[a, b]$  into smaller subintervals and use Simpson's rule on each subinterval, see figure 12.5b. Note though that Simpson's rule is not quite like the other numerical integration techniques we have studied when it comes to splitting the interval into smaller pieces: The interval over which  $f$  is to be integrated is split into subintervals, and Simpson's rule is applied on neighbouring *pairs* of intervals, see figure 12.6. In other words, each parabola is defined over *two* subintervals which means that the total number of subintervals must be even, and the number of given values of  $f$  must be odd.

If the partition is  $\{x_i\}_{i=0}^{2n}$  with  $x_i = a + ih$ , Simpson's rule on the interval

$[x_{2i-2}, x_{2i}]$  is

$$\int_{x_{2i-2}}^{x_{2i}} f(x) dx \approx \frac{h}{3} (f(x_{2i-2}) + 4f(x_{2i-1}) + f(x_{2i})).$$

The approximation of the total integral is therefore

$$\int_a^b f(x) dx \approx \frac{h}{3} \sum_{i=1}^n (f(x_{2i-2}) + 4f(x_{2i-1}) + f(x_{2i})).$$

In this sum we observe that the right endpoint of one subinterval becomes the left endpoint of the neighbouring subinterval to the right. Therefore, if this is implemented directly, the function values at the points with an even subscript will be evaluated twice, except for the extreme endpoints  $a$  and  $b$  which only occur once in the sum. We can therefore rewrite the sum in a way that avoids these redundant evaluations.

**Observation 12.14.** Suppose  $f$  is a function defined on the interval  $[a, b]$ , and let  $\{x_i\}_{i=0}^{2n}$  be a uniform partition of  $[a, b]$  with step length  $h$ . The composite Simpson's rule approximates the integral of  $f$  by

$$\int_a^b f(x) dx \approx I_{\text{Simp}}(h) = \frac{h}{3} \left( f(a) + f(b) + 2 \sum_{i=1}^{n-1} f(x_{2i}) + 4 \sum_{i=1}^n f(x_{2i-1}) \right).$$

With the midpoint rule, we computed a sequence of approximations to the integral by successively halving the width of the subintervals. The same is often done with Simpson's rule, but then care should be taken to avoid unnecessary function evaluations since all the function values computed at one step will also be used at the next step.

**Example 12.15.** Let us test Simpson's rule on the same example as the midpoint rule and the trapezoidal rule,

$$\int_0^1 \cos x dx = \sin 1 \approx 0.8414709848.$$

As in example 12.6, we split the interval into  $2^k$  subintervals, for  $k = 1, 2, \dots, 10$ .

The result is

$h$	$I_{\text{Simp}}(h)$	Error
0.250000	0.84148938	$-1.8 \times 10^{-5}$
0.125000	0.84147213	$-1.1 \times 10^{-6}$
0.062500	0.84147106	$-7.1 \times 10^{-8}$
0.031250	0.84147099	$-4.5 \times 10^{-9}$
0.015625	0.84147099	$-2.7 \times 10^{-10}$
0.007813	0.84147098	$-1.7 \times 10^{-11}$
0.003906	0.84147098	$-1.1 \times 10^{-12}$
0.001953	0.84147098	$-6.8 \times 10^{-14}$
0.000977	0.84147098	$-4.3 \times 10^{-15}$
0.000488	0.84147098	$-2.2 \times 10^{-16}$

where the error is defined by

$$\int_0^1 f(x) dx - I_{\text{Simp}}(h).$$

When we compare this table with examples 12.6 and 12.10, we note that the error is now much smaller. We also note that each time the step length is halved, the error is reduced by a factor of 16. In other words, by introducing one more function evaluation in each subinterval, we have obtained a method with much better accuracy. This will be quite evident when we analyse the error below. ■

### 12.4.3 The error

An expression for the error in Simpson's rule can be derived by using the same technique as for the previous methods: We replace  $f(x)$ ,  $f(a)$  and  $f(b)$  by cubic Taylor polynomials with remainders about the point  $a_{1/2}$ , and then collect and simplify terms. However, these computations become quite long and tedious, and as for the trapezoidal rule, the constant in the error term is not the best possible. We therefore just state the best possible error estimate here without proof.

**Lemma 12.16** (Local error). *If  $f$  is continuous and has continuous derivatives up to order 4 on the interval  $[a, b]$ , the error in Simpson's rule is bounded by*

$$|E(f)| \leq \frac{(b-a)^5}{2880} \max_{x \in [a,b]} |f^{(iv)}(x)|.$$

We note that the error in Simpson's rule depends on  $(b-a)^5$ , while the error in the midpoint rule and trapezoidal rule depend on  $(b-a)^3$ . This means that

the error in Simpson's rule goes to zero much more quickly than for the other two methods when the width of the interval  $[a, b]$  is reduced.

### The global error

The approach we used to deduce the global error for the midpoint rule, see theorem 12.8, can also be used to derive the global error in Simpson's rule. The following theorem sums this up.

**Theorem 12.17** (Global error). *Suppose that  $f$  and its first 4 derivatives are continuous on the interval  $[a, b]$ , and that the integral of  $f$  on  $[a, b]$  is approximated by Simpson's rule with  $2n$  subintervals of equal width  $h$ . Then the error is bounded by*

$$|E(f)| \leq (b-a) \frac{h^4}{2880} \max_{x \in [a,b]} |f^{(iv)}(x)|. \quad (12.23)$$

The estimate (12.23) explains the behaviour we noticed in example 12.15: Because of the factor  $h^4$ , the error is reduced by a factor  $2^4 = 16$  when  $h$  is halved, and for this reason, Simpson's rule is a very popular method for numerical integration.

### Exercises

- 1 Calculate an approximation to the integral

$$\int_0^{\pi/2} \frac{\sin x}{1+x^2} dx = 0.526978557614\dots$$

with Simpson's rule. Split the interval into 6 subintervals.

- 2 a) How many function evaluations do you need to calculate the integral

$$\int_0^1 \frac{dx}{1+2x}$$

with the trapezoidal rule to make sure that the error is smaller than  $10^{-10}$ .

- b) How many function evaluations are necessary to achieve the same accuracy with the midpoint rule?
- c) How many function evaluations are necessary to achieve the same accuracy with Simpson's rule?
- 3 In this exercise you are going to program an algorithm like algorithm 12.5 for Simpson's rule. If you cannot program, use Simpson's rule manually with 10 subintervals, check the error, and skip the second part of (b).

- a) Write a program that implements Simpson's rule as in algorithm 12.5 and test it on the integral

$$\int_0^1 e^x dx = e - 1.$$

- b) Determine a value of  $h$  that guarantees that the absolute error is smaller than  $10^{-10}$ . Run your program and check what the actual error is for this value of  $h$ . (You may have to adjust algorithm 12.5 slightly and print the absolute error.)
- 4 a) Verify that Simpson's rule is exact when  $f(x) = x^i$  for  $i = 0, 1, 2, 3$ .  
 b) Use (a) to show that Simpson's rule is exact for any cubic polynomial.  
 c) Could you reach the same conclusion as in (b) by just considering the error estimate (12.23)?

- 5 We want to design a numerical integration method

$$\int_a^b f(x) dx \approx w_1 f(a) + w_2 f(a_{1/2}) + w_3 f(b).$$

Determine the unknown coefficients  $w_1$ ,  $w_2$ , and  $w_3$  by demanding that the integration method should be exact for the three polynomials  $f(x) = x^i$  for  $i = 0, 1, 2$ . Do you recognise the method?

## 12.5 Summary

In this chapter we have derived three methods for numerical integration. All these methods and their error analyses may seem rather overwhelming, but they all follow a common thread:

**Procedure 12.18.** *The following is a general procedure for deriving numerical methods for integration of a function  $f$  over the interval  $[a, b]$ :*

1. *Interpolate the function  $f$  by a polynomial  $p$  at suitable points.*
2. *Approximate the integral of  $f$  by the integral of  $p$ . This makes it possible to express the approximation to the integral in terms of function values of  $f$ .*
3. *Derive an estimate for the local error by expanding the function values in Taylor series with remainders about the midpoint  $a_{1/2} = (a + b)/2$ .*
4. *Derive an estimate for the global error by using the technique leading up to theorem 12.8.*