Numerical Integration 31.2

Introduction

In this Section we will present some methods that can be used to approximate integrals. Attention will be paid to how we ensure that such approximations can be guaranteed to be of a certain level of accuracy.

Prerequisites

Before starting this Section you should ...

- review previous material on integrals and integration

Learning Outcomes

On completion you should be able to ...

- approximate certain integrals
- be able to ensure that these approximations are of some desired accuracy

1. Numerical integration

The aim in this Section is to describe numerical methods for approximating integrals of the form

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

One motivation for this is in the material on probability that appears in HELM 39. Normal distributions can be analysed by working out

$$\int_a^b \frac{1}{\sqrt{2\pi}}\,e^{-x^2/2}\,dx$$

for certain values of a and b. It turns out that it is not possible, using the kinds of functions most engineers would care to know about, to write down a function with derivative equal to $\frac{1}{\sqrt{2\pi}}\,e^{-x^2/2}$ so values of the integral are approximated instead. Tables of numbers giving the value of this integral for different interval widths appeared at the end of HELM 39, and it is known that these tables are accurate to the number of decimal places given. How can this be known? One aim of this Section is to give a possible answer to that question.

It is clear that, not only do we need a way of approximating integrals, but we also need a way of working out the accuracy of the approximations if we are to be sure that our tables of numbers are to be relied on.

In this Section we address both of these points, begining with a simple approximation method.

2. The simple trapezium rule

The first approximation we shall look at involves finding the area under a straight line, rather than the area under a curve f. Figure 6 shows it best.

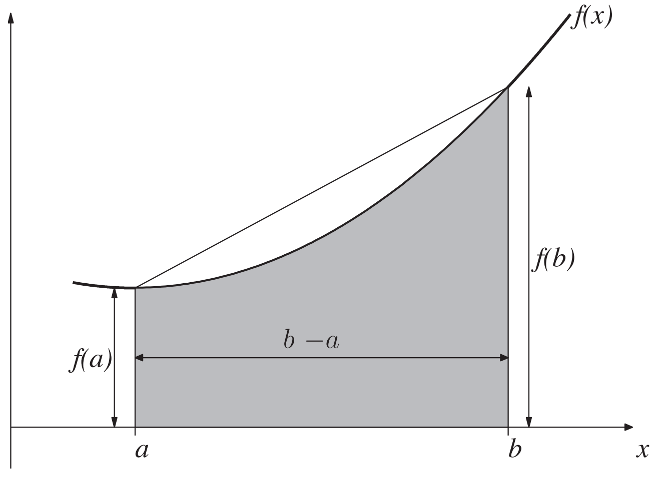

Figure 6

We approximate as follows

$$\begin{aligned}\int_a^b f(x)\,dx &= \text{grey shaded area}\\ &\approx \text{area of the trapezium surrounding the shaded region}\\ &= \text{width of trapezium} \times \text{average height of the two sides}\\ &= \frac{1}{2}(b-a)\Big(f(a)+f(b)\Big)\end{aligned}$$

Key Point 5

Simple Trapezium Rule

The simple trapezium rule for approximating $\displaystyle\int_a^b f(x)\,dx$ is given by approximating the area under the graph of f by the area of a trapezium.

The formula is:

$$\int_a^b f(x)\,dx \approx \frac{1}{2}(b-a)\big(f(a)+f(b)\big)$$

Or, to put it another way that may prove helpful a little later on,

$$\int_a^b f(x)\,dx \approx \frac{1}{2} \times (\text{interval width}) \times \Big(\ f(\text{left-hand end}) \quad + \quad f(\text{right-hand end})\ \Big)$$

Next we show some instances of implementing this method.

Example 10

Approximate each of these integrals using the simple trapezium rule

(a) $\displaystyle\int_0^{\pi/4} \sin(x)\,dx$ (b) $\displaystyle\int_1^2 e^{-x^2/2}\,dx$ (c) $\displaystyle\int_0^2 \cosh(x)\,dx$

Solution

(a) $\displaystyle\int_0^{\pi/4} \sin(x)\,dx \approx \frac{1}{2}(b-a)(\sin(a)+\sin(b)) = \frac{1}{2}\left(\frac{\pi}{4}-0\right)\left(0+\frac{1}{\sqrt{2}}\right) = 0.27768,$

(b) $\displaystyle\int_1^2 e^{-x^2/2}\,dx \approx \frac{1}{2}(b-a)\left(e^{-a^2/2}+e^{-b^2/2}\right) = \frac{1}{2}(1-0)\left(e^{-1/2}+e^{-2}\right) = 0.37093,$

(c) $\displaystyle\int_0^2 \cosh(x)\,dx \approx \frac{1}{2}(b-a)(\cosh(a)+\cosh(b)) = \frac{1}{2}(2-0)(1+\cosh(2)) = 4.76220,$

where all three answers are given to 5 decimal places.

It is important to note that, although we have given these integral approximations to 5 decimal places, this does not mean that they are accurate to that many places. We will deal with the accuracy of our approximations later in this Section. Next are some Tasks for you to try.

Task

Approximate the following integrals using the simple trapezium method

(a) $\displaystyle\int_1^5 \sqrt{x}\,dx$ (b) $\displaystyle\int_1^2 \ln(x)\,dx$

Your solution

Answer

(a) $\displaystyle\int_1^5 \sqrt{x}\,dx \approx \frac{1}{2}(b-a)\left(\sqrt{a}+\sqrt{b}\right) = \frac{1}{2}(5-1)\left(1+\sqrt{5}\right) = 6.47214$

(b) $\displaystyle\int_1^2 \ln(x)\,dx \approx \frac{1}{2}(b-a)(\ln(a)+\ln(b)) = \frac{1}{2}(1-0)\,(0+\ln(2)) = 0.34657$

The answer you obtain for this next Task can be checked against the table of results in HELM 39 concerning the Normal distribution or in a standard statistics textbook.

Task

Use the simple trapezium method to approximate $\displaystyle\int_0^1 \frac{1}{\sqrt{2\pi}}\,e^{-x^2/2}\,dx$

Your solution

Answer

We find that

$$\int_0^1 \frac{1}{\sqrt{2\pi}}\,e^{-x^2/2}\,dx \approx \frac{1}{2}(1-0)\frac{1}{\sqrt{2\pi}}(1+e^{-1/2}) = 0.32046$$

to 5 decimal places.

So we have a means of approximating $\displaystyle\int_a^b f(x)\,dx$. The question remains whether or not it is a *good* approximation.

How good is the simple trapezium rule?

We define e_T, the error in the simple trapezium rule to be the difference between the actual value of the integral and our approximation to it, that is

$$e_T = \int_a^b f(x)\,dx \quad - \quad \frac{1}{2}(b-a)\Big(f(a)+f(b)\Big)$$

It is enough for our purposes here to omit some theory and skip straight to the result of interest. In many different textbooks on the subject it is shown that

$$e_T = -\frac{1}{12}(b-a)^3 f''(c)$$

where c is some number between a and b. (The principal drawback with this expression for e_T is that we do not know what c is, but we will find a way to work around that difficulty later.)

It is worth pausing to ask what meaning we can attach to this expression for e_T. There are two factors which can influence e_T:

1. If $b-a$ is small then, clearly, e_T will most probably also be small. This seems sensible enough - if the integration interval is a small one then there is "less room" to accumulate a large error. (This observation forms part of the motivation for the composite trapezium rule discussed later in this Section.)

2. If f'' is small everywhere in $a < x < b$ then e_T will be small. This reflects the fact that we worked out the integral of a straight line function, instead of the integral of f. If f is a long way from being a straight line then f'' will be large and so we must expect the error e_T to be large too.

We noted above that the expression for e_T is less useful than it might be because it involves the unknown quantity c. We perform a trade-off to get around this problem. The expression above gives an exact value for e_T, but we do not know enough to evaluate it. So we replace the expression with one we *can* evaluate, but it will not be exact. We replace $f''(c)$ with a worst case value to obtain an **upper bound** on e_T. This worst case value is the largest (positive or negative) value that $f''(x)$ achieves for $a \le x \le b$. This leads to

$$|e_T| \le \max_{a\le x\le b}\Big|f''(x)\Big|\,\frac{(b-a)^3}{12}.$$

We summarise this in Key Point 6.

Key Point 6

Error in the Simple Trapezium Rule

The error, $|e_T|$, in the simple trapezium approximation to $\displaystyle\int_a^b f(x)\,dx$ is bounded above by

$$\max_{a\le x\le b}\Big|f''(x)\Big|\,\frac{(b-a)^3}{12}$$

Example 11

Work out the error bound (to 6 decimal places) for the simple trapezium method approximations to

(a) $\displaystyle\int_0^{\pi/4} \sin(x)\,dx$ (b) $\displaystyle\int_0^2 \cosh(x)\,dx$

Solution

In each case the trickiest part is working out the maximum value of $f''(x)$.

(a) Here $f(x) = \sin(x)$, therefore $f'(x) = -\cos(x)$ and $f''(x) = -\sin(x)$. The function $\sin(x)$ takes values between 0 and $\frac{1}{\sqrt{2}}$ when x varies between 0 and $\pi/4$. Hence

$$e_T < \frac{1}{\sqrt{2}} \times \frac{(\pi/4)^3}{12} = 0.028548 \quad \text{to 6 decimal places.}$$

(b) If $f(x) = \cosh(x)$ then $f''(x) = \cosh(x)$ too. The maximum value of $\cosh(x)$ for x between 0 and 2 will be $\cosh(2) = 3.762196$, to 6 decimal places. Hence, in this case,

$$e_T < (3.762196) \times \frac{(2-0)^3}{12} = 2.508130 \quad \text{to 6 decimal places.}$$

(In Example 11 we used a rounded value of $\cosh(2)$. To be on the safe side, it is best to round this number *up* to make sure that we still have an upper bound on e_T. In this case, of course, rounding up is what we would naturally do, because the seventh decimal place was a 6.)

Task

Work out the error bound (to 5 significant figures) for the simple trapezium method approximations to

(a) $\displaystyle\int_1^5 \sqrt{x}\,dx$ (b) $\displaystyle\int_1^2 \ln(x)\,dx$

Your solution

(a)

Answer

If $f(x) = \sqrt{x} = x^{1/2}$ then $f'(x) = \frac{1}{2}x^{-1/2}$ and $f''(x) = -\frac{1}{4}x^{-3/2}$.

The negative power here means that f'' takes its biggest value in magnitude at the left-hand end of the interval $[1, 5]$ and we see that $\max_{1 \leq x \leq 5} |f''(x)| = f''(1) = \frac{1}{4}$. Therefore

$$e_T < \frac{1}{4} \times \frac{4^3}{12} = 1.3333 \quad \text{to 5 s.f.}$$

Your solution

(b)

Answer

Here $f(x) = \ln(x)$ hence $f'(x) = 1/x$ and $f''(x) = -1/x^2$.

It follows then that $\max_{1 \leq x \leq 2} |f''(x)| = 1$ and we conclude that

$$e_T < 1 \times \frac{1^3}{12} = 0.083333 \quad \text{to 5 s.f.}$$

One deficiency in the simple trapezium rule is that there is nothing we can do to improve it. Having computed an error bound to measure the quality of the approximation we have no way to go back and work out a better approximation to the integral. It would be preferable if there were a parameter we could alter to tune the accuracy of the method. The following approach uses the simple trapezium method in a way that allows us to improve the accuracy of the answer we obtain.

3. The composite trapezium rule

The general idea here is to split the interval $[a, b]$ into a sequence of N smaller subintervals of equal width $h = (b - a)/N$. Then we apply the simple trapezium rule to each of the subintervals.

Figure 7 below shows the case where $N = 2$ (and $\therefore\ h = \frac{1}{2}(b - a)$). To simplify notation later on we let $f_0 = f(a)$, $f_1 = f(a + h)$ and $f_2 = f(a + 2h) = f(b)$.

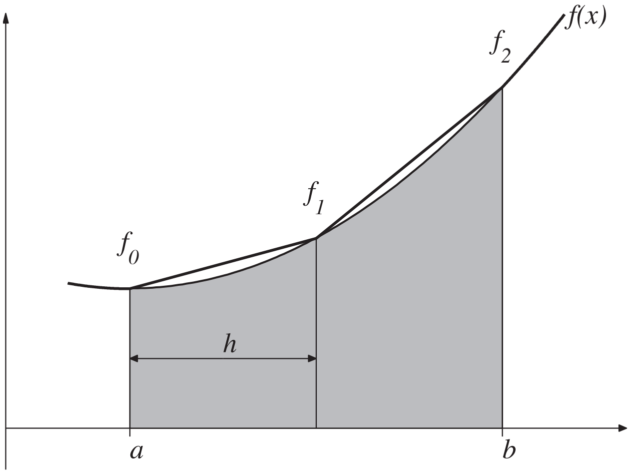

Figure 7

Applying the simple trapezium rule to each subinterval we get

$$\begin{aligned}\int_a^b f(x)\,dx &\approx \text{(area of first trapezium)} + \text{(area of second trapezium)}\\ &= \frac{1}{2}h(f_0 + f_1) + \frac{1}{2}h(f_1 + f_2) = \frac{1}{2}h\left(f_0 + 2f_1 + f_2\right)\end{aligned}$$

where we remember that the width of each of the subintervals is h, rather than the $b - a$ we had in the simple trapezium rule.

The next improvement will come from taking $N = 3$ subintervals (Figure 8). Here $h = \frac{1}{3}(b - a)$ is smaller than in Figure 7 above and we denote $f_0 = f(a)$, $f_1 = f(a + h)$, $f_2 = f(a + 2h)$ and $f_3 = f(a + 3h) = f(b)$. (Notice that f_1 and f_2 mean something different from what they did in the $N = 2$ case.)

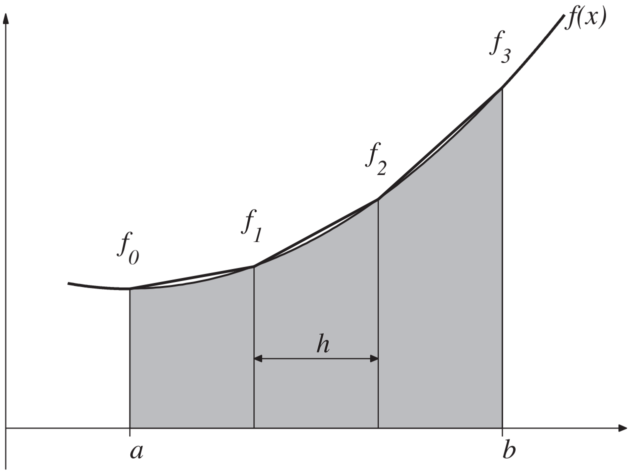

Figure 8

As Figure 8 shows, the approximation is getting closer to the grey shaded area and in this case we have

$$\begin{aligned}\int_a^b f(x)\,dx &\approx \frac{1}{2}h(f_0+f_1)+\frac{1}{2}h(f_1+f_2)+\frac{1}{2}h(f_2+f_3)\\ &= \frac{1}{2}h\Big(f_0\ +2\{f_1+f_2\}+\ f_3\Big).\end{aligned}$$

The pattern is probably becoming clear by now, but here is one more improvement. In Figure 9 $N=4$, $h=\frac{1}{4}(b-a)$ and we denote $f_0=f(a)$, $f_1=f(a+h)$, $f_2=f(a+2h)$, $f_3=f(a+3h)$ and $f_4=f(a+4h)=f(b)$.

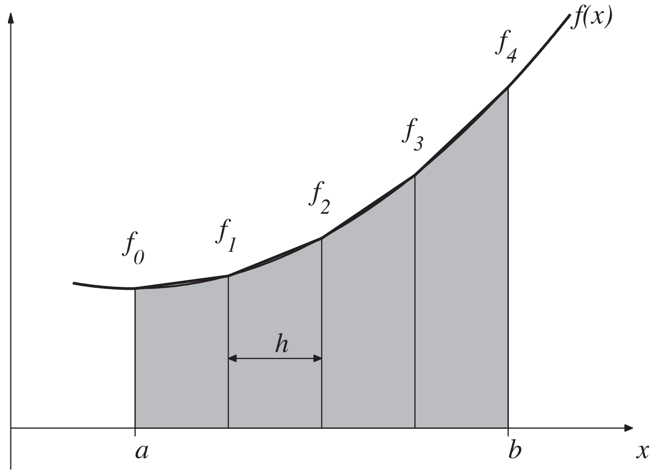

Figure 9

This leads to

$$\begin{aligned}\int_a^b f(x)\,dx &\approx \frac{1}{2}h(f_0+f_1)+\frac{1}{2}h(f_1+f_2)+\frac{1}{2}h(f_2+f_3)++\frac{1}{2}h(f_3+f_4)\\ &= \frac{1}{2}h\Big(f_0\ +2\{f_1+f_2+f_3\}+\ f_4\Big).\end{aligned}$$

We generalise this idea into the following Key Point.

Key Point 7

Composite Trapezium Rule

The composite trapezium rule for approximating $\int_a^b f(x)\,dx$ is carried out as follows:

1. Choose N, the number of subintervals,

2. $\displaystyle\int_a^b f(x)\,dx \approx \frac{1}{2}h\left(f_0 \;+2\{f_1+f_2+\cdots+f_{N-1}\}+\; f_N\right),$

   where

$$h=\frac{b-a}{N}, \qquad f_0=f(a),\quad f_1=f(a+h),\ldots,f_n=f(a+nh),\ldots,$$
$$\text{and}\quad f_N=f(a+Nh)=f(b).$$

Example 12

Using 4 subintervals in the composite trapezium rule, and working to 6 decimal places, approximate

$$\int_0^2 \cosh(x)\,dx$$

Solution

In this case $h=(2-0)/4=0.5$.
We require $\cosh(x)$ evaluated at five x-values and the results are tabulated below to 6 d.p.

x_n	$f_n=\cosh(x_n)$
0	1.000000
0.5	1.127626
1	1.543081
1.5	2.352410
2	3.762196

It follows that

$$\begin{aligned}\int_0^2 \cosh(x)\,dx &\approx \frac{1}{2}h\left(f_0+f_4+2\{f_1+f_2+f_3\}\right)\\ &= \frac{1}{2}(0.5)\left(1+3.762196+2\{1.127626+1.543081+2.35241\}\right)\\ &= 3.452107\end{aligned}$$

Task

Using 4 subintervals in the composite trapezium rule approximate

$$\int_1^2 \ln(x)\, dx$$

Your solution

Answer

In this case $h = (2-1)/4 = 0.25$.

We require $\ln(x)$ evaluated at five x-values and the results are tabulated below t0 6 d.p.

x_n	$f_n = \ln(x_n)$
1	0.000000
1.25	0.223144
1.5	0.405465
1.75	0.559616
2	0.693147

It follows that

$$\begin{aligned}\int_1^2 \ln(x)\, dx &\approx \frac{1}{2}h\left(f_0 + f_4 + 2\{f_1 + f_2 + f_3\}\right)\\ &= \frac{1}{2}(0.25)\left(0 + 0.693147 + 2\{0.223144 + 0.405465 + 0.559616\}\right)\\ &= 0.383700\end{aligned}$$

How good is the composite trapezium rule?

We can work out an upper bound on the error incurred by the composite trapezium method. Fortunately, all we have to do here is apply the method for the error in the simple rule over and over again. Let e_T^N denote the error in the composite trapezium rule with N subintervals. Then

$$\begin{aligned} \left|e_T^N\right| &\leq \max_{\text{1st subinterval}} \left|f''(x)\right| \frac{h^3}{12} + \max_{\text{2nd subinterval}} \left|f''(x)\right| \frac{h^3}{12} + \ldots + \max_{\text{last subinterval}} \left|f''(x)\right| \frac{h^3}{12} \\ &= \frac{h^3}{12} \underbrace{\left(\max_{\text{1st subinterval}} \left|f''(x)\right| + \max_{\text{2nd subinterval}} \left|f''(x)\right| + \ldots + \max_{\text{last subinterval}} \left|f''(x)\right| \right)}_{N \text{ terms}}. \end{aligned}$$

This is all very well as a piece of theory, but it is awkward to use in practice. The process of working out the maximum value of $|f''|$ separately in each subinterval is very time-consuming. We can obtain a more user-friendly, if less accurate, error bound by replacing each term in the last bracket above with the biggest one. Hence we obtain

$$\left|e_T^N\right| \leq \frac{h^3}{12}\left(N \max_{a \leq x \leq b} \left|f''(x)\right| \right)$$

This upper bound can be rewritten by recalling that $Nh = b - a$, and we now summarise the result in a Key Point.

Key Point 8

Error in the Composite Trapezium Rule

The error, $\left|e_T^N\right|$, in the N-subinterval composite trapezium approximation to $\displaystyle\int_a^b f(x)\,dx$ is bounded above by

$$\max_{a \leq x \leq b} \left|f''(x)\right| \frac{(b-a)h^2}{12}$$

Note: the special case when $N = 1$ is the simple trapezium rule, in which case $b - a = h$ (refer to Key Point 6 to compare).

The formula in Key Point 8 can be used to decide how many subintervals to use to guarantee a specific accuracy.

Example 13

The function f is known to have a second derivative with the property that

$$|f''(x)| < 12$$

for x between 0 and 4.

Using the error bound given in Key Point 8 determine how many subintervals are required so that the composite trapezium rule used to approximate

$$\int_0^4 f(x)\,dx$$

can be guaranteed to be in error by less than $\frac{1}{2} \times 10^{-3}$.

Solution

We require that

$$12 \times \frac{(b-a)h^2}{12} < 0.0005$$

that is

$$4h^2 < 0.0005.$$

This implies that $h^2 < 0.000125$ and therefore $h < 0.0111803$.
Now $N = (b-a)/h = 4/h$ and it follows that

$$N > 357.7708$$

Clearly, N must be a whole number and we conclude that the smallest number of subintervals which *guarantees* an error smaller than 0.0005 is $N = 358$.

It is worth remembering that the error bound we are using here is a pessimistic one. We effectively use the same (worst case) value for $f''(x)$ all the way through the integration interval. Odds are that fewer subintervals will give the required accuracy, but the value for N we found here will guarantee a good enough approximation.

Next are two Tasks for you to try.

Task

The function f is known to have a second derivative with the property that

$$|f''(x)| < 14$$

for x between -1 and 4.

Using the error bound given in Key Point 8 determine how many subintervals are required so that the composite trapezium rule used to approximate

$$\int_{-1}^{4} f(x)\, dx$$

can be guaranteed to have an error less than 0.0001.

Your solution

Answer

We require that

$$14 \times \frac{(b-a)h^2}{12} < 0.0001$$

that is

$$\frac{70h^2}{12} < 0.0001$$

This implies that $h^2 < 0.00001714$ and therefore $h < 0.0041404$.
Now $N = (b-a)/h = 5/h$ and it follows that

$$N > 1207.6147$$

Clearly, N must be a whole number and we conclude that the smallest number of subintervals which *guarantees* an error smaller than 0.00001 is $N = 1208$.

Task

It is given that the function $e^{-x^2/2}$ has a second derivative that is never greater than 1 in absolute value.

(a) Use this fact to determine how many subintervals are required for the composite trapezium method to deliver an approximation to

$$\int_0^1 \frac{1}{\sqrt{2\pi}}\, e^{-x^2/2}\, dx$$

that is guaranteed to have an error less than $\frac{1}{2} \times 10^{-2}$.

(b) Find an approximation to the integral that is in error by less than $\frac{1}{2} \times 10^{-2}$.

Your solution

(a)

Answer

We require that $\dfrac{1}{\sqrt{2\pi}}\dfrac{(b-a)h^2}{12} < 0.005$. This means that $h^2 < 0.150398$ and therefore, since $N = 1/h$, it is necessary for $N = 3$ for the error bound to be less than $\pm\frac{1}{2} \times 10^{-2}$.

Your solution

(b)

Answer

To carry out the composite trapezium rule, with $h = \frac{1}{3}$ we need to evaluate $f(x) = \dfrac{1}{\sqrt{2\pi}}\, e^{-x^2/2}$ at $x = 0,\ h,\ 2h,\ 1$. This evaluation gives

$$f(0) = f_0 = 0.39894, \qquad f(h) = f_1 = 0.37738, \qquad f(2h) = f_2 = 0.31945$$

$$\text{and} \qquad f(1) = f_3 = 0.24197,$$

all to 5 decimal places. It follows that

$$\int_0^1 \frac{1}{\sqrt{2\pi}}\, e^{-x^2/2}\, dx \approx \frac{1}{2}h(f_0 + f_3 + 2\{f_1 + f_2\}) = 0.33910$$

We know from part (a) that this approximation is in error by less than $\frac{1}{2} \times 10^{-2}$.

Example 14

Determine the minimum number of steps needed to guarantee an error not exceeding ± 0.001, when evaluating

$$\int_0^1 \cosh(x^2)\, dx$$

using the trapezium rule.

Solution

$$f(x) = \cosh(x^2) \qquad f'(x) = 2x\sinh(x^2) \qquad f''(x) = 2\sinh(x^2) + 4x^2\cosh(x^2)$$

Using the error formula in Key Point 8

$$E = \left| -\frac{1}{12}h^2\{2\sinh(x^2) + 4x^2\cosh(x^2)\} \right| \qquad x \in [0, 1]$$

$|E|_{\mathsf{max}}$ occurs when $x = 1$

$$\begin{aligned}
0.001 &> \frac{h^2}{12}\{2\sinh(1) + 4\cosh(1)\} \\
h^2 &< 0.012/\{(2\sinh(1) + 4\cosh(1)\} \\
\Rightarrow h^2 &< 0.001408 \\
\Rightarrow h &< 0.037523 \\
\Rightarrow n &\geq 26.651 \\
\Rightarrow n &= 27 \quad \text{needed}
\end{aligned}$$

Task

Determine the minimum of strips, n, needed to evaluate by the trapezium rule:

$$\int_0^{\pi/4} \{3x^2 - 1.5\sin(2x)\}\, dx$$

such that the error is guaranteed not to exceed ± 0.005.

Your solution

Answer

$f(x) = 3x^2 - 1.5\sin(2x) \qquad f''(x) = 6 + 6\sin(2x)$

|Error| will be maximum at $x = \dfrac{\pi}{4}$ so that $\sin(2x) = 1$

$$E = -\frac{(b-a)}{12}h^2 f^{(2)}(x) \qquad x \in [0, \frac{\pi}{4}]$$

$$E = -\frac{\pi}{48}h^2 6\{1 + \sin(2x)\}, \qquad x \in [0, \frac{\pi}{4}]$$

$$|E|_{\mathsf{max}} = \frac{\pi}{48}h^2(12) = \frac{\pi h^2}{4}$$

We need $\dfrac{\pi h^2}{4} < 0.005 \qquad \Rightarrow h^2 < \dfrac{0.02}{\pi} \qquad \Rightarrow \qquad h < 0.07979$

Now $nh = (b-a) = \dfrac{\pi}{4}$ so $n = \dfrac{\pi}{4h}$

We need $n > \dfrac{\pi}{4 \times 0.07979} = 9.844$ so $n = 10$ required

4. Other methods for approximating integrals

Here we briefly describe other methods that you may have heard, or get to hear, about. In the end they all amount to the same sort of thing, that is we sample the integrand f at a few points in the integration interval and then take a weighted average of all these f values. All that is needed to implement any of these methods is the list of sampling points and the weight that should be attached to each evaluation. Lists of these points and weights can be found in many books on the subject.

Simpson's rule

This is based on passing a quadratic through three equally spaced points, rather than passing a straight line through two points as we did for the simple trapezium rule. The composite Simpson's rule is given in the following Key Point.

Key Point 9

Composite Simpson's Rule

The composite Simpson's rule for approximating $\displaystyle\int_a^b f(x)\,dx$ is carried out as follows:

1. Choose N, which must be an $\boxed{\text{even}}$ number of subintervals,

2. Calculate $\displaystyle\int_a^b f(x)\,dx$

$$\approx \tfrac{1}{3}h\left(f_0 \ + 4\{f_1 + f_3 + f_5 + \cdots + f_{N-1}\} + 2\{f_2 + f_4 + f_6 + \cdots + f_{N-2}\} + \ f_N\right)$$

where

$$h = \frac{b-a}{N}, \qquad f_0 = f(a), \quad f_1 = f(a+h), \ldots, f_n = f(a+nh), \ldots,$$
$$\text{and} \quad f_N = f(a+Nh) = f(b).$$

The formula in Key Point 9 is slightly more complicated than the corresponding one for composite trapezium rule. One way of remembering the rule is the learn the pattern

$$1 \ \ 4 \ \ 2 \ \ 4 \ \ 2 \ \ 4 \ \ 2 \ \ \ldots \ \ 4 \ \ 2 \ \ 4 \ \ 2 \ \ 4 \ \ 1$$

which show that the end point values are multiplied by 1, the values with odd-numbered subscripts are multiplied by 4 and the *interior* values with even subscripts are multiplied by 2.

Example 15

Using 4 subintervals in the composite Simpson's rule approximate

$$\int_0^2 \cosh(x)\,dx.$$

Solution

In this case $h = (2-0)/4 = 0.5$.
We require $\cosh(x)$ evaluated at five x-values and the results are tabulated below to 6 d.p.

x_n	$f_n = \cosh(x_n)$
0	1.000000
0.5	1.127626
1	1.543081
1.5	2.352410
2	3.762196

It follows that

$$\begin{aligned}\int_0^2 \cosh(x)\,dx &\approx \frac{1}{3}h\,(f_0 + 4f_1 + 2f_2 + 4f_3 + f_4)\\ &= \frac{1}{3}(0.5)\,(1 + 4\times 1.127626 + 2\times 1.543081 + 4\times 2.352410 + 3.762196)\\ &= 3.628083,\end{aligned}$$

where this approximation is given to 6 decimal places.

This approximation to $\displaystyle\int_0^2 \cosh(x)\;dx$ is closer to the true value of $\sinh(2)$ (which is 3.626860 to 6 d.p.) than we obtained when using the composite trapezium rule with the same number of subintervals.

Task

Using 4 subintervals in the composite Simpson's rule approximate

$$\int_1^2 \ln(x)\,dx.$$

Your solution

Answer

In this case $h = (2-1)/4 = 0.25$. There will be five x-values and the results are tabulated below to 6 d.p.

x_n	$f_n = \ln(x_n)$
1.00	0.000000
1.25	0.223144
1.50	0.405465
1.75	0.559616
2.00	0.693147

It follows that

$$\begin{aligned}\int_1^2 \ln(x)\,dx &\approx \frac{1}{3}h\,(f_0 + 4f_1 + 2f_2 + 4f_3 + f_4)\\ &= \frac{1}{3}(0.25)\,(0 + 4\times 0.223144 + 2\times 0.405465 + 4\times 0.559616 + 0.693147)\\ &= 0.386260 \quad \text{to 6 d.p.}\end{aligned}$$

How good is the composite Simpson's rule?

On page 39 (Key Point 8) we saw a formula for an upper bound on the error in the composite trapezium method. A corresponding result for the composite Simpson's rule exists and is given in the following Key Point.

Key Point 10

Error in Composite Simpson's Rule

The error in the N-subinterval composite Simpson's rule approximation to $\displaystyle\int_a^b f(x)\,dx$ is bounded above by

$$\max_{a\le x\le b}\left|f^{(iv)}(x)\right|\frac{(b-a)h^4}{180}$$

(Here $f^{(iv)}$ is the fourth derivative of f and h is the subinterval width, so $N \times h = b - a$.)

The formula in Key Point 10 can be used to decide how many subintervals to use to guarantee a specific accuracy.

Example 16

The function f is known to have a fourth derivative with the property that

$$\left|f^{(iv)}(x)\right| < 5$$

for x between 1 and 5. Determine how many subintervals are required so that the composite Simpson's rule used to approximate

$$\int_1^5 f(x)\,dx$$

incurs an error that is guaranteed less than 0.005 .

Solution

We require that

$$5 \times \frac{4h^4}{180} < 0.005$$

This implies that $h^4 < 0.045$ and therefore $h < 0.460578$.
Now $N = 4/h$ and it follows that

$$N > 8.684741$$

For the composite Simpson's rule N must be an *even* whole number and we conclude that the smallest number of subintervals which *guarantees* an error smaller than 0.005 is $N = 10$.

Task

The function f is known to have a fourth derivative with the property that

$$\left|f^{(iv)}(x)\right| < 12$$

for x between 2 and 6. Determine how many subintervals are required so that the composite Simpson's rule used to approximate

$$\int_2^6 f(x)\,dx$$

incurs an error that is guaranteed less than 0.0005 .

Your solution

Answer
We require that

$$12 \times \frac{4h^4}{180} < 0.0005$$

This implies that $h^4 < 0.001875$ and therefore $h < 0.208090$.
Now $N = 4/h$ and it follows that

$$N > 19.222491$$

N must be an *even* whole number and we conclude that the smallest number of subintervals which *guarantees* an error smaller than 0.0005 is $N = 20$.

The following Task is similar to one that we saw earlier in this Section (page 42). Using the composite Simpson's rule we can achieve greater accuracy, for a similar amount of effort, than we managed using the composite trapezium rule.

Task

It is given that the function $e^{-x^2/2}$ has a fourth derivative that is never greater than 3 in absolute value.

(a) Use this fact to determine how many subintervals are required for the composite Simpson's rule to deliver an approximation to

$$\int_0^1 \frac{1}{\sqrt{2\pi}}\, e^{-x^2/2}\, dx$$

that is guaranteed to have an error less than $\frac{1}{2} \times 10^{-4}$.

Your solution

Answer
We require that $\dfrac{3}{\sqrt{2\pi}} \dfrac{(b-a)h^4}{180} < 0.00005$.

This means that $h^4 < 0.00751988$ and therefore $h < 0.294478$. Since $N = 1/h$ it is necessary for $N = 4$ for the error bound to be guaranteed to be less than $\pm\frac{1}{2} \times 10^{-4}$.

(b) Find an approximation to the integral that is in error by less than $\frac{1}{2} \times 10^{-4}$.

Your solution

Answer

In this case $h = (1-0)/4 = 0.25$. We require $\dfrac{1}{\sqrt{2\pi}}\, e^{-x^2/2}$ evaluated at five x-values and the results are tabulated below to 6 d.p.

x_n	$\dfrac{1}{\sqrt{2\pi}}\, e^{-x_n^2/2}$
0	0.398942
0.25	0.386668
0.5	0.352065
0.75	0.301137
1	0.241971

It follows that

$$\begin{aligned}
\int_0^1 \frac{1}{\sqrt{2\pi}}\, e^{-x^2/2}\, dx &\approx \frac{1}{3}h\,(f_0 + 4f_1 + 2f_2 + 4f_3 + f_4) \\
&= \frac{1}{3}(0.25)\,(0.398942 + 4 \times 0.386668 + 2 \times 0.352065 \\
&\qquad + 4 \times 0.301137 + 0.241971) \\
&= 0.341355 \quad \text{to 6 d.p.}
\end{aligned}$$

We know from part (a) that this approximation is in error by less than $\frac{1}{2} \times 10^{-4}$

Example 17

Find out how many strips are needed to be sure that

$$\int_0^4 \sinh(2t)\, dt$$

is evaluated by Simpson's rule with error less than ± 0.0001

Solution

$$E = -\frac{(b-a)}{180} h^4 (16) \sinh(2x) \qquad 0 < x < 4$$

$$|E| \leq \frac{64h^2 \sinh(8)}{180} \leq 0.0001$$

$$\Rightarrow h^4 \leq \frac{0.0180}{64 \sinh(8)} \Rightarrow h \leq 0.0208421$$

$$nh = b - a \quad \Rightarrow \quad n \geq \frac{4}{0.0208421} = 191.92$$

So $n = 192$ is needed (minimum even number).

Engineering Example 1

Plastic bottle design

Introduction

Manufacturing containers is a large and varied industry and optimum packaging can save companies millions of pounds. Although determining the capacity of a container and amount of material needed can be done by physical experiment, mathematical modelling provides a cost-effective and efficient means for the designer to experiment.

Problem in words

A manufacturer is designing a new plastic bottle to contain 900 ml of fabric softener. The bottle is circular in cross section, with a varying radius given by

$$r = 4 + 0.5z - 0.07z^2 + 0.002z^3$$

where z is the height above the base in cm.

(a) Find an expression for the volume of the bottle and hence show that the fill level needs to be approximately 18 cm.

(b) If the wall thickness of the plastic is 1 mm, show that this is always small compared to the bottle radius.

(c) Hence, find the volume of plastic required to manufacture a bottle which is 20 cm tall (include the plastic in the base and side walls), using a numerical method.

A graph the radius against z is shown below:

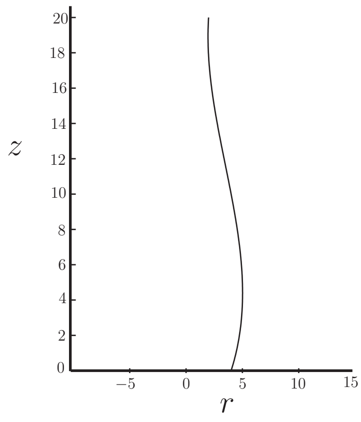

Figure 10

Mathematical statement of problem

Calculate all lengths in centimetres.

(a) The formula for the volume of a solid of revolution, revolved round the z axis between $z = 0$ and $z = d$ is $\int_0^d \pi r^2 \, dz$. We have to evaluate this integral.

(b) To show that the thickness is small relative to the radius we need to find the minimum radius.

(c) Given that the thickness is small compared with the radius, the volume can be taken to be the surface area times the thickness. Now the surface area of the base is easy to calculate being $\pi \times 4^2$, but we also need to calculate the surface area for the sides, which is much harder.

For an element of height dz this is $2\pi z\times$(the slant height) of the surface between z and $z+dz$. The slant height is, analytically $\left(\sqrt{1+\left(\dfrac{dr}{dz}\right)^2}\right) \times dz$, or equivalently the distance between $(r(z), z)$ and $(r(z+dz), z+dz)$, which is easier to use numerically.

Analytically the surface area to height 20 is $\displaystyle\int_0^{20} 2\pi r\sqrt{1+\left(\frac{dr}{dz}\right)^2}\; dz$; we shall approximate this numerically. This will give the area of the side surface.

Mathematical analysis

(a) We could calculate this integral exactly, as the volume is $\displaystyle\int_0^d \pi(4+0.5z-0.07z^2+0.002z^3)^2\, dz$ but here we do this numerically (which can often be a simpler approach and possibly is so here). To do that we need to keep an eye on the likely error, and for this problem we shall ensure the error in the integrals is less than 1 ml. The formula for the error with the trapezium rule, with step h and integrated from 0 to 20 (assuming from the problem that we shall not integrate over a larger range) is $\dfrac{20}{12}h^2\text{max}|f''|$. Doing this crudely with $f = \pi g^2$ where $g(z) = 4+0.5z-0.07z^2+0.002z^3$ we see that

$$|g(z)| \leq 4+10+28+16 = 58 \quad \text{(using only positive signs and } |z| \leq 20)$$

and $\quad |g'(z)| \leq 0.5+0.14z+0.006z^2 \leq 0.5+2.8+2.4 = 5.7 < 6,$

and $\quad |g''(z)| \leq 0.14+0.012z \leq 0.38.$

Therefore

$$f'' = 2\pi(gg''+(g')^2) \leq 2(58\times 0.38+6^2)\pi < 117\pi, \quad \text{so} \quad \frac{20}{12}h^2\text{max}|f''| \leq 613h^2.$$

We need $h^2 < 1/613$, or $h < 0.0403$. We will use $h = 0.02$, and the error will be at most 0.25.

The approximation to the integral from 0 to 18 is

$$\frac{1}{2}\pi g^2(0)0.02 + \sum_{i=1}^{899}\pi g^2(0.02i)0.02 + \frac{1}{2}\pi g^2(18)0.02$$

(recalling the multiplying factor is a half for the first and last entries in the trapezium rule). This yields a value of 899.72, which is certainly within 1 ml of 900.

(b) From the graph the minimum radius looks to be about 2 at about $z = 18$. Looking more exactly (found by solving the quadratic to find the places where the derivative is zero, or by plotting the values and by inspection), the minimum is at $z = 18.93$, when $r = 1.948$ cm. So the thickness is indeed small (always less than 0.06 of the radius at all places.)

(c) For the area of the side surface we shall calculate $\displaystyle\int_0^{20} 2\pi r\sqrt{1+\left(\frac{dr}{dz}\right)^2}\,dz$ numerically, using the trapezium rule with step 0.02 as before. $\displaystyle\sqrt{1+\left(\frac{dr}{dz}\right)^2}\,dz = \sqrt{(dz)^2+(dr)^2}$, which we shall approximate at point z_n by $\sqrt{(z_{n+1}-z_n)^2+(r_{n+1}-r_n)^2}$, so evaluating $r(z)$ at intervals of 0.02 gives the approximation

$$\pi r(0)\sqrt{(0.02)^2+(r(0.02)-r(0))^2}+\sum_{i=1}^{999} 2\pi r(0.02i)\sqrt{(0.02)^2+(r(0.02(i+1))-r(0.02i))^2}$$

$$+\pi r(20)\sqrt{(0.02)^2+(r(20)-r(19.98))^2}.$$

Calculating this gives 473 cm^2. Approximating the analytical expression by a direct numerical calculation gives 474 cm^2. (The answer is between 473.5 and 473.6 cm^2, so this variation is understandable and does not indicate an error.) The bottom surface area is $16\pi = 50.3$ cm^2, so the total surface area we may take to be $474+50 = 524$ cm^2, and hence the volume of plastic is $524\times 0.1 = 52.4$ cm^3.

Mathematical comment

An alternative to using the trapezium rule is Simpson's rule which will require many fewer steps.

When using a computer program such as Microsoft Excel having an efficient method may not be important for a small problem but could be significant when many calculations are needed or computational power is limited (such as if using a programmable calculator).

The reader is invited to repeat the calculations for (a) and (c) using Simpson's rule.

The analytical answer to (a) is given by

$$\int_0^{18} \pi(16+4z-0.31z^2-0.054z^3+0.0069z^4-0.00028z^5+0.000004z^6)\,dz$$

which gives 899.7223 to 4 d.p.

Exercises

1. Using 4 subintervals in the composite trapezium rule approximate

$$\int_1^5 \sqrt{x}\,dx.$$

2. The function f is known to have a second derivative with the property that

$$|f''(x)| < 12$$

for x between 2 and 3. Using the error bound given earlier in this Section determine how many subintervals are required so that the composite trapezium rule used to approximate

$$\int_2^3 f(x)\,dx$$

can be guaranteed to have an error in it that is less than 0.001.

3. Using 4 subintervals in the composite Simpson rule approximate

$$\int_1^5 \sqrt{x}\,dx.$$

4. The function f is known to have a fourth derivative with the property that

$$\left|f^{(iv)}(x)\right| < 6$$

for x between -1 and 5 . Determine how many subintervals are required so that the composite Simpson's rule used to approximate

$$\int_{-1}^5 f(x)\,dx$$

incurs an error that is less than 0.001.

5. Determine the minimum number of steps needed to guarantee an error not exceeding ± 0.000001 when numerically evaluating

$$\int_2^4 \ln(x)\,dx$$

using Simpson's rule.

Answers

1. In this case $h = (5-1)/4 = 1$. We require $\sqrt{x}$ evaluated at five x-values and the results are tabulated below

x_n	$f_n = \sqrt{x_n}$
1	1
2	1.414214
3	1.732051
4	2.000000
5	2.236068

It follows that

$$\begin{aligned}\int_1^5 \sqrt{x}\,dx &\approx \frac{1}{2}h\left(f_0 + f_4 + 2\{f_1 + f_2 + f_3\}\right)\\ &= \frac{1}{2}(1)\Big(1 + 2.236068 + 2\{1.414214 + 1.732051 + 2\}\Big)\\ &= 6.764298.\end{aligned}$$

2. We require that $12 \times \dfrac{(b-a)h^2}{12} < 0.001$. This implies that $h < 0.0316228$.
Now $N = (b-a)/h = 1/h$ and it follows that

$$N > 31.6228$$

Clearly, N must be a whole number and we conclude that the smallest number of subintervals which *guarantees* an error smaller than 0.001 is $N = 32$.

3. In this case $h = (5-1)/4 = 1$.
We require $\sqrt{x}$ evaluated at five x-values and the results are as tabulated in the solution to Exercise 1. It follows that

$$\begin{aligned}\int_1^5 \sqrt{x}\,dx &\approx \frac{1}{3}h\left(f_0 + 4f_1 + 2f_2 + 4f_3 + f_4\right)\\ &= \frac{1}{3}(1)\left(1 + 4\times 1.414214 + 2\times 1.732051 + 4\times 2.000000 + 2.236068\right)\\ &= 6.785675.\end{aligned}$$

4. We require that $6 \times \dfrac{6h^4}{180} < 0.001$. This implies that $h^4 < 0.005$ and therefore $h < 0.265915$. Now $N = 6/h$ and it follows that $N > 22.563619$. We know that N must be an *even* whole number and we conclude that the smallest number of subintervals which *guarantees* an error smaller than 0.001 is $N = 24$.

Answers

5. $f(x) = \ln(x) \qquad f^{(4)}(x) = -\dfrac{6}{x^4}$

$$\text{Error} = -\frac{(b-a)h^4 f^{(4)}(x)}{180} \qquad a = 2,\ b = 4$$

$$|E| = \frac{2h^4(6/x^4)}{180} \qquad x \in [2,4]$$

$$|E|_{\text{max}} = \frac{h^4}{15}\frac{1}{2^4} \leq 0.000001$$

$$\Rightarrow h^4 \leq 15 \times 2^4 \times 0.000001 \Rightarrow h \leq 0.124467$$

Now $nh = (b-a)$ so

$$n \geq \frac{2}{0.124467} \Rightarrow n \geq 16.069568 \Rightarrow n = 18 \quad \text{(minimum even number)}$$