FIRST YEAR CALCULUS

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Chapter 11

NUMERICAL INTEGRATION

11.1. Introduction

In Chapters 9 and 10, we have discussed some analytic techniques for evaluating integrals. However, many integrals that arise in science and engineering resist attack by even the most sophisticated analytic techniques. In such instances, we may have to accept a rather poor and perhaps even not entirely satisfactory second best, and attempt to make reasonable approximations by numerical techniques.

11.2. The Trapezium Rule

Suppose that we wish to evaluate an integral

$$\int_A^B f(x)\,\mathrm{d}x,$$

where the function $f(x)$ is finite and continuous in the closed interval $[A,B]$. If we draw the curve $y=f(x)$, then the value of the integral is the same as the area bounded by the curve $y=f(x)$ and the lines $y=0$, $x=A$ and $x=B$ (the reader should draw a diagram).

A first, and rather crude, approximation to the integral is to take the area of the trapezium with vertices at the points $(A,0)$, $(B,0)$, $(A,f(A))$ and $(B,f(B))$. In other words, we take the approximation

$$\int_A^B f(x)\,\mathrm{d}x \approx \frac{1}{2}(B-A)(f(A)+f(B)). \tag{1}$$

In practice, however, we take more points than just A and B. Consider the dissection

$$A = x_0 < x_1 < \ldots < x_n = B$$

of the interval $[A, B]$. Clearly we have

$$\int_A^B f(x)\,\mathrm{d}x = \sum_{i=1}^{n} \int_{x_{i-1}}^{x_i} f(x)\,\mathrm{d}x.$$

Suppose now that we make a similar approximation as (1) in each of the subintervals, so that for every $i = 1, \ldots, n$, we have

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

Then we have the approximation

$$\int_A^B f(x)\,\mathrm{d}x \approx \frac{1}{2}\sum_{i=1}^{n}(x_i - x_{i-1})(f(x_{i-1}) + f(x_i)). \tag{2}$$

Suppose further that the lengths of all the subintervals are the same, so that

$$x_i - x_{i-1} = h = \frac{B - A}{n} \quad \text{for every } i = 1, \ldots, n.$$

Then (2) becomes

$$\int_A^B f(x)\,\mathrm{d}x \approx \frac{h}{2}(f(x_0) + 2f(x_1) + 2f(x_2) + \ldots + 2f(x_{n-1}) + f(x_n)).$$

This is called the Trapezium rule for n intervals.

EXAMPLE 11.2.1. We wish to estimate the value of $\log 2$ by a Trapezium rule approximation to the integral

$$\int_1^2 \frac{1}{x}\,\mathrm{d}x.$$

Then $f(x) = 1/x$ in the interval $[1, 2]$. If we take $h = 1/2$, then we have

x	1	$\frac{3}{2}$	2
$f(x)$	1	$\frac{2}{3}$	$\frac{1}{2}$

and so

$$\int_1^2 \frac{1}{x}\,\mathrm{d}x \approx \frac{1}{4}\left(1 + \frac{4}{3} + \frac{1}{2}\right) = 0.7083 \text{ (4dp)}.$$

If we take $h = 1/4$, then we have

x	1	$\frac{5}{4}$	$\frac{3}{2}$	$\frac{7}{4}$	2
$f(x)$	1	$\frac{4}{5}$	$\frac{2}{3}$	$\frac{4}{7}$	$\frac{1}{2}$

and so

$$\int_1^2 \frac{1}{x}\,\mathrm{d}x \approx \frac{1}{8}\left(1 + \frac{8}{5} + \frac{4}{3} + \frac{8}{7} + \frac{1}{2}\right) = 0.6970 \text{ (4dp)}.$$

11.3. The Midpoint Rule

This method is fundamentally similar to the Trapezium rule. Suppose that we wish to evaluate an integral

$$\int_A^B f(x)\,\mathrm{d}x,$$

where the function $f(x)$ is finite and continuous in the closed interval $[A,B]$.

Consider the point $C=\frac{1}{2}(A+B)$, the midpoint in the interval $[A,B]$ (the reader should draw a diagram). We take the approximation

$$\int_A^B f(x)\,\mathrm{d}x \approx (B-A)f\left(\frac{A+B}{2}\right). \tag{3}$$

Suppose that we divide the interval $[A,B]$ into n subintervals by the dissection

$$A=x_0<x_1<\ldots<x_n=B,$$

and make a similar approximation as (3) in each of the subintervals, so that for every $i=1,\ldots,n$, we have

$$\int_{x_{i-1}}^{x_i} f(x)\,\mathrm{d}x \approx (x_i-x_{i-1})f\left(\frac{x_{i-1}+x_i}{2}\right).$$

Then we have the approximation

$$\int_A^B f(x)\,\mathrm{d}x \approx \sum_{i=1}^{n}(x_i-x_{i-1})f\left(\frac{x_{i-1}+x_i}{2}\right). \tag{4}$$

Suppose further that the lengths of all the subintervals are the same, so that

$$x_i-x_{i-1}=h=\frac{B-A}{n}\quad\text{for every } i=1,\ldots,n.$$

Then (4) becomes

$$\int_A^B f(x)\,\mathrm{d}x \approx h\sum_{i=1}^{n} f\left(\frac{x_{i-1}+x_i}{2}\right).$$

This is called the Midpoint rule for n intervals.

EXAMPLE 11.3.1. We wish to estimate the value of $\log 2$ by a Midpoint rule approximation to the integral

$$\int_1^2 \frac{1}{x}\,\mathrm{d}x.$$

Then $f(x)=1/x$ in the interval $[1,2]$. If we take $h=1/2$, then we have

x	(1)	$\frac{5}{4}$	$(\frac{3}{2})$	$\frac{7}{4}$	(2)
$f(x)$		$\frac{4}{5}$		$\frac{4}{7}$	

and so

$$\int_1^2 \frac{1}{x}\,\mathrm{d}x \approx \frac{1}{2}\left(\frac{4}{5}+\frac{4}{7}\right) = 0.6857 \text{ (4dp)}.$$

If we take $h = 1/4$, then we have

x	(1)	$\frac{9}{8}$	$(\frac{5}{4})$	$\frac{11}{8}$	$(\frac{3}{2})$	$\frac{13}{8}$	$(\frac{7}{4})$	$\frac{15}{8}$	(2)
$f(x)$		$\frac{8}{9}$		$\frac{8}{11}$		$\frac{8}{13}$		$\frac{8}{15}$	

and so

$$\int_1^2 \frac{1}{x}\,\mathrm{d}x \approx \frac{1}{4}\left(\frac{8}{9}+\frac{8}{11}+\frac{8}{13}+\frac{8}{15}\right) = 0.6912 \text{ (4dp)}.$$

11.4. Simpson's Rule

Suppose that we wish to evaluate an integral

$$\int_A^B f(x)\,\mathrm{d}x,$$

where the function $f(x)$ is finite and continuous in the closed interval $[A,B]$.

In both the Trapezium rule and the Midpoint rule, a crude approximation to the area under the curve is obtained by replacing the curve between $x = A$ and $x = B$ by a straight line segment; in other words, a polynomial of degree 1. A natural extension of this idea is to replace the curve by a parabola; in other words, a polynomial of degree 2, passing through the points $(A, f(A))$, $(B, f(B))$ and $(C, f(C))$, where $C = \frac{1}{2}(A+B)$.

Consider first the simple case $A = -H$ and $B = H$, so that $C = 0$. We wish to fit a parabola

$$p(x) = \alpha x^2 + \beta x + \gamma$$

through these points. Then

$$\begin{aligned} \alpha H^2 - \beta H + \gamma &= f(-H), \\ \gamma &= f(0), \\ \alpha H^2 + \beta H + \gamma &= f(H), \end{aligned}$$

so that

$$\begin{aligned} \alpha &= \frac{f(-H) - 2f(0) + f(H)}{2H^2}, \\ \beta &= \frac{f(H) - f(-H)}{2H}, \\ \gamma &= f(0). \end{aligned}$$

We now take the approximation

$$\int_{-H}^{H} f(x)\,\mathrm{d}x \approx \int_{-H}^{H} (\alpha x^2 + \beta x + \gamma)\,\mathrm{d}x = \frac{2}{3}\alpha H^3 + 2\gamma H = \frac{H}{3}(f(-H) + 4f(0) + f(H)).$$

In general, if we wish to use this approximation over the interval $[A, B]$, the above becomes

$$\int_A^B f(x)\,\mathrm{d}x \approx \frac{B-A}{6}\left(f(A) + 4f\left(\frac{A+B}{2}\right) + f(B)\right).$$

This is called Simpson's rule with 3 ordinates.

Similar to the Trapezium rule and the Midpoint rule, we may apply Simpson's rule on subintervals of the interval $[A, B]$. Suppose that we divide the interval $[A, B]$ into n subintervals by the dissection

$$A = x_0 < x_1 < \ldots < x_n = B,$$

where n is even and

$$x_i - x_{i-1} = h = \frac{B-A}{n} \quad \text{for every } i = 1, \ldots, n.$$

Applying Simpson's rule to the interval $[x_{2j-2}, x_{2j}]$, we have

$$\int_{x_{2j-2}}^{x_{2j}} f(x)\,\mathrm{d}x \approx \frac{x_{2j} - x_{2j-2}}{6}(f(x_{2j-2}) + 4f(x_{2j-1}) + f(x_{2j})),$$

so that

$$\int_A^B f(x)\,\mathrm{d}x \approx \frac{h}{3}\left(f(x_0) + f(x_n) + 4\sum_{\substack{i=1\\ i \text{ odd}}}^{n-1} f(x_i) + 2\sum_{\substack{i=1\\ i \text{ even}}}^{n-1} f(x_i)\right).$$

This is called Simpson's rule for $(n+1)$ ordinates, where n is even. Note that the coefficients for

$$f(x_0), f(x_1), f(x_2), \ldots, f(x_n)$$

are respectively

$$1, 4, 2, 4, 2, 4, 2, \ldots, 4, 2, 4, 1.$$

Example 11.4.1. We wish to estimate the value of $\log 2$ by a Simpson rule approximation to the integral

$$\int_1^2 \frac{1}{x}\,\mathrm{d}x.$$

Then $f(x) = 1/x$ in the interval $[1, 2]$. If we take $h = 1/2$, hence 3 ordinates, then we have

x	1	$\frac{3}{2}$	2
$f(x)$	1	$\frac{2}{3}$	$\frac{1}{2}$

and so

$$\int_1^2 \frac{1}{x}\,\mathrm{d}x \approx \frac{1}{6}\left(1 + \frac{8}{3} + \frac{1}{2}\right) = 0.6944 \text{ (4dp)}.$$

If we take $h = 1/4$, hence 5 ordinates, then we have

x	1	$\frac{5}{4}$	$\frac{3}{2}$	$\frac{7}{4}$	2
$f(x)$	1	$\frac{4}{5}$	$\frac{2}{3}$	$\frac{4}{7}$	$\frac{1}{2}$

and so

$$\int_1^2 \frac{1}{x}\,\mathrm{d}x \approx \frac{1}{12}\left(1+\frac{16}{5}+\frac{4}{3}+\frac{16}{7}+\frac{1}{2}\right) = 0.6933 \text{ (4dp)}.$$

11.5. Truncation Errors

In this section, we state without proof some results concerning the errors that inevitably occur when we apply the Trapezium rule, Midpoint rule or Simpson's rule. As far as numerical integration is concerned, such error analysis is more important than the estimates that are given by the rules. The study of these questions forms part of numerical analysis.

For the Trapezium rule and Midpoint rule, we have the following two results.

PROPOSITION 11A. *Suppose that the function $f(x)$ is finite and continuous in the closed interval $[A,B]$, and that the second derivative $f''(x)$ exists for every $x \in (A,B)$. Suppose further that the Trapezium rule, applied to the dissection*

$$A = x_0 < x_1 < \ldots < x_n = B$$

of $[A,B]$ into n subintervals, where

$$x_i - x_{i-1} = h = \frac{B-A}{n} \quad \text{for every } i = 1, \ldots, n,$$

gives rise to the error

$$T_n = \int_A^B f(x)\,\mathrm{d}x - \frac{h}{2}(f(x_0) + 2f(x_1) + 2f(x_2) + \ldots + 2f(x_{n-1}) + f(x_n)).$$

Then

$$|T_n| \le \frac{K(B-A)^3}{12n^2} = \frac{K(B-A)h^2}{12},$$

where

$$K = \max_{x\in[A,B]} |f''(x)|.$$

Furthermore, if $f''(x)$ does not change sign in the interval $[A,B]$, then T_n has the opposite sign to the sign of $f''(x)$ in this interval.

PROPOSITION 11B. *Suppose that the function $f(x)$ is finite and continuous in the closed interval $[A,B]$, and that the second derivative $f''(x)$ exists for every $x \in (A,B)$. Suppose further that the Midpoint rule, applied to the dissection*

$$A = x_0 < x_1 < \ldots < x_n = B$$

of $[A,B]$ into n subintervals, where

$$x_i - x_{i-1} = h = \frac{B-A}{n} \quad \text{for every } i = 1, \ldots, n,$$

gives rise to the error

$$M_n = \int_A^B f(x)\,\mathrm{d}x - h\sum_{i=1}^{n} f\left(\frac{x_{i-1}+x_i}{2}\right).$$

Then

$$|M_n| \le \frac{K(B-A)^3}{24n^2} = \frac{K(B-A)h^2}{24},$$

where

$$K = \max_{x\in[A,B]} |f''(x)|.$$

Furthermore, if $f''(x)$ does not change sign in the interval $[A,B]$, then M_n has the same sign as the sign of $f''(x)$ in this interval.

Example 11.5.1. In our Trapezium and Midpoint rule approximation to $\log 2$, we have used the function $f(x) = 1/x$ in the interval $[1,2]$. Note that $f''(x) = 2/x^3 > 0$ in this interval. It follows that $T_n < 0$ and $M_n > 0$. This means that our Trapezium rule estimates are over-estimates, and our Midpoint rule estimates are under-estimates.

The corresponding result for Simpson's rule is somewhat different.

PROPOSITION 11C. *Suppose that the function $f(x)$ is finite and continuous in the closed interval $[A,B]$, and that the fourth derivative $f''''(x)$ exists for every $x \in (A,B)$. Suppose further that Simpson's rule, applied to the dissection*

$$A = x_0 < x_1 < \ldots < x_n = B$$

of $[A,B]$ into n subintervals, where n is even and

$$x_i - x_{i-1} = h = \frac{B-A}{n} \quad \text{for every } i = 1,\ldots,n,$$

gives rise to the error

$$S_n = \int_A^B f(x)\,\mathrm{d}x - \frac{h}{3}\left(f(x_0) + f(x_n) + 4\sum_{\substack{i=1\\ i\text{ odd}}}^{n-1} f(x_i) + 2\sum_{\substack{i=1\\ i\text{ even}}}^{n-1} f(x_i)\right).$$

Then

$$|S_n| \le \frac{L(B-A)^5}{180n^4} = \frac{L(B-A)h^4}{180},$$

where

$$L = \max_{x\in[A,B]} |f''''(x)|.$$

Furthermore, if $f''''(x)$ does not change sign in the interval $[A,B]$, then S_n has the opposite sign to the sign of $f''''(x)$ in this interval.

Example 11.5.2. In our Simpson rule approximation to $\log 2$, we have used the function $f(x) = 1/x$ in the interval $[1,2]$. Note that $f''''(x) = 24/x^5 > 0$ in this interval. It follows that $S_n < 0$. This means that our estimates are over-estimates.

11.6. Richardson Extrapolation

Throughout, we assume that the function $f(x)$ is continuous in the closed interval $[A,B]$, and write

$$I=\int_A^B f(x)\,\mathrm{d}x.$$

Consider first of all the Trapezium rule. Suppose that $f''(x)$ does not change sign in the interval $[A,B]$. Suppose further that $T(h)$ denotes the Trapezium rule approximation to I with a given h. Then in view of Proposition 11A, we have

$$I-T(h)\approx C_T(B-A)h^2,$$

where C_T is a constant, so that

$$\frac{I-T(h)}{h^2}\approx C_T(B-A).$$

Repeating the same argument on the Trapezium rule approximation to I with $h/2$, we have

$$\frac{I-T(h/2)}{(h/2)^2}\approx C_T(B-A).$$

It follows that

$$\frac{I-T(h)}{h^2}\approx\frac{I-T(h/2)}{(h/2)^2},$$

so that $I-T(h)\approx 4(I-T(h/2))$, whence

$$I\approx\frac{4T(h/2)-T(h)}{3}.$$

Example 11.6.1. Recall our estimates of $\log 2$ in Example 11.2.1. We have

$$T(1/2)=0.7083\text{ (4dp)}\qquad\text{and}\qquad T(1/4)=0.6970\text{ (4dp)}.$$

Hence

$$I\approx\frac{4(0.6970)-(0.7083)}{3}\approx 0.6932.$$

Consider next the Midpoint rule. Suppose that $f''(x)$ does not change sign in the interval $[A,B]$. Suppose further that $M(h)$ denotes the Midpoint rule approximation to I with a given h. Then in view of Proposition 11B, we have

$$I-M(h)\approx C_M(B-A)h^2,$$

where C_M is a constant, so that

$$\frac{I-M(h)}{h^2}\approx C_M(B-A).$$

Repeating the same argument on the Midpoint rule approximation to I with $h/2$, we have

$$\frac{I-M(h/2)}{(h/2)^2}\approx C_M(B-A).$$

It follows that

$$\frac{I - M(h)}{h^2} \approx \frac{I - M(h/2)}{(h/2)^2},$$

so that $I - M(h) \approx 4(I - M(h/2))$, whence

$$I \approx \frac{4M(h/2) - M(h)}{3}.$$

EXAMPLE 11.6.2. Recall our estimates of $\log 2$ in Example 11.3.1. We have

$$M(1/2) = 0.6857 \text{ (4dp)} \qquad \text{and} \qquad M(1/4) = 0.6912 \text{ (4dp)}.$$

Hence

$$I \approx \frac{4(0.6912) - (0.6857)}{3} \approx 0.6930.$$

Consider finally Simpson's rule. Suppose that $f''''(x)$ does not change sign in the interval $[A, B]$. Suppose further that $S(h)$ denotes the Simpson rule approximation to I with a given h. Then in view of Proposition 11C, we have

$$I - S(h) \approx C_S(B - A)h^4,$$

where C_S is a constant, so that

$$\frac{I - S(h)}{h^4} \approx C_S(B - A).$$

Repeating the same argument on the Simpson rule approximation to I with $h/2$, we have

$$\frac{I - S(h/2)}{(h/2)^4} \approx C_S(B - A).$$

It follows that

$$\frac{I - S(h)}{h^4} \approx \frac{I - S(h/2)}{(h/2)^4},$$

so that $I - S(h) \approx 16(I - S(h/2))$, whence

$$I \approx \frac{16S(h/2) - S(h)}{15}.$$

EXAMPLE 11.6.3. Recall our estimates of $\log 2$ in Example 11.4.1. We have

$$S(1/2) = 0.6944 \text{ (4dp)} \qquad \text{and} \qquad S(1/4) = 0.6933 \text{ (4dp)}.$$

Hence

$$I \approx \frac{16(0.6933) - (0.6944)}{15} \approx 0.6932.$$

REMARK. It is worth noting that $\log 2 = 0.6931$ (4dp).

Problems for Chapter 11

1. Consider the integral $\displaystyle\int_0^1 \frac{1}{1+x^2}\,\mathrm{d}x$.

   a) Find the Trapezium rule approximation with 2 intervals.
   b) Find the Trapezium rule approximation with 4 intervals.
   c) Find the Midpoint rule approximation with 2 intervals.
   d) Find the Midpoint rule approximation with 4 intervals.
   e) Discuss whether the estimates in (a)–(d) are over-estimates or under-estimates. Justify your assertions.
   f) Find the Simpson rule approximation with 2 intervals.
   g) Find the Simpson rule approximation with 4 intervals.
   h) Use Richardson extrapolation on your results in (a)–(d).
   i) What number are we approximating?