Chapter 4

Numerical integration

Contents

4.1 Definite integrals

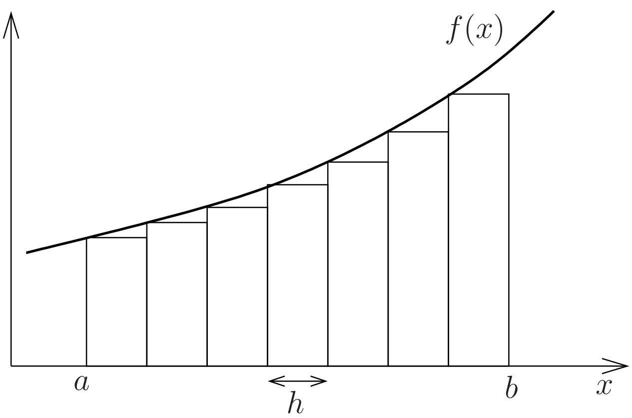
The definite integral of a function f on the interval $[a, b]$ is written as

$$\int_a^b f(x)\,\mathrm{d}x \tag{4.1}$$

and can be defined as the limit of the Riemann series

$$\int_a^b f(x)\,\mathrm{d}x = \lim_{h\to 0} \sum_{i=1}^{(b-a)/h} hf(a + (i-1)h),$$

i.e. <u>as the area under the curve</u> $(x, y = f(x))$.



Hence, numerical integration is often called quadrature (i.e. computation of an area under a curve).

The definite integral of a function exists even if there is no analytic antiderivative function $F(x)$ such that

$$\frac{\mathrm{d}}{\mathrm{d}x}F(x) = f(x).$$

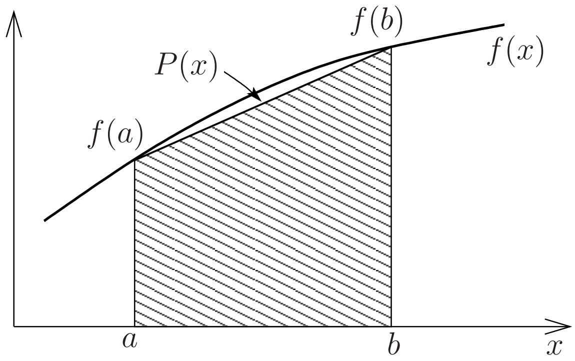
4.2 Closed Newton-Cotes formulae

The definite integral (4.1) can be approximated using the polynomial interpolating $f(x)$ through n equispaced points (x_k), leading to

$$\int_a^b f(x)\,\mathrm{d}x \approx \sum_{k=1}^{n} w_k f(x_k) \quad \text{with} \quad x_k = a + (k-1)\frac{b-a}{n-1}.$$

4.2.1 Trapezium rule

This is the simplest numerical method for evaluating a definite integral. It calculates the area of the trapezium formed by approximating $f(x)$ using linear interpolation.



$$\int_a^b f(x)\,\mathrm{d}x \approx \frac{b-a}{2}\left(f(a)+f(b)\right). \tag{4.2}$$

Thus, the trapezium rule can be obtained by integrating the linear interpolation function

$$P(x) = f(a)\frac{x-b}{a-b} + f(b)\frac{x-a}{b-a} \quad \text{over the interval } [a,b].$$

(Check that $\int_a^b f(x)\,\mathrm{d}x \approx \int_a^b P(x)\,\mathrm{d}x$ leads to (4.2).)

Measure of the error: From Equation (3.4), we know the error in the linear interpolation,

$$f(x) = P(x) + \frac{1}{2}f''(\xi(x))(x-a)(x-b), \quad \xi(x) \in [a,b].$$

Therefore,

$$\int_a^b f(x)\,\mathrm{d}x = \int_a^b P(x)\,\mathrm{d}x + \int_a^b \frac{1}{2}f''(\xi(x))(x-a)(x-b)\,\mathrm{d}x.$$

So, the error in the trapezium rule is equal to

$$E = \frac{1}{2}\int_a^b f''(\xi(x))(x-a)(x-b)\,\mathrm{d}x.$$

To evaluate this integral, we shall make use of the following theorem (generalisation of the Mean Value Theorem).

Theorem 4.1 (Weighted Mean Value for Integrals)
If $h \in C[a,b]$, if the integral of $g(x)$ exists on $[a,b]$, and if $g(x)$ does not change sign on $[a,b]$, then there exists $c \in [a,b]$ such that

$$\int_a^b h(x)g(x)\,\mathrm{d}x = h(c)\int_a^b g(x)\,\mathrm{d}x.$$

Hence,

$$\frac{1}{2}\int_a^b f''(\xi(x))(x-a)(x-b)\,\mathrm{d}x = \frac{f''(c)}{2}\int_a^b (x-a)(x-b)\,\mathrm{d}x$$

since $(x-a)(x-b) \leq 0$ on the interval $[a,b]$.

$$\begin{aligned} E &= \frac{1}{2}f''(c)\int_0^{b-a} u(u-(b-a))\,\mathrm{d}u \quad \text{with } u = x-a, \\ &= \frac{1}{2}f''(c)\left[\frac{u^3}{3} - \frac{u^2}{2}(b-a)\right]_0^{b-a} = -f''(c)\frac{(b-a)^3}{12}. \end{aligned}$$

Thus, the error in the trapezium method scales with the cube of the size on the interval. (Note that this method is exact for linear functions.)

We can generate other integration rules by using higher order Lagrange polynomials.

$$\begin{aligned} \int_a^b f(x)\,\mathrm{d}x \approx \int_a^b P(x)\,\mathrm{d}x &= \int_a^b \sum_{k=1}^n f(x_k)L_k(x)\,\mathrm{d}x \\ &= \sum_{k=1}^n f(x_k)\int_a^b L_k(x)\,\mathrm{d}x = \sum_{k=1}^n w_k f(x_k), \end{aligned}$$

where $w_k = \displaystyle\int_a^b L_k(x)\,\mathrm{d}x$ are called <u>weights</u>.
The error is given by $\displaystyle\int_a^b \frac{f^{(n)}(\xi(x))}{n!}\prod_{k=1}^n (x-x_k)\,\mathrm{d}x$.
This method provides a means of finding the weights and error terms. However, their evaluation becomes more and more complex with increasing n. (Theorem 4.1 cannot be used to evaluate the error since $\displaystyle\prod_{k=1}^n (x-x_k)$ changes sign for $n \geq 3$.)

4.2.2 Method of undetermined coefficients

Alternative way of evaluating Newton-Cotes integration formulae. To illustrate this method, let us derive the trapezium rule again.

Trapezium rule

We wish to find an approximation of the form

$$\int_a^b f(x)\,\mathrm{d}x \approx w_1 f(a) + w_2 f(b).$$

Since, we have two unknown parameters, w_1 and w_2, we can make this formulae exact for linear functions (i.e. functions are of the form $\alpha x + \beta$). So, the error term must be of the form $Kf''(\xi)$ for some $\xi \in (a,b)$.

Hence, we seek a quadrature rule of the form

$$\int_a^b f(x)\,\mathrm{d}x = w_1 f(a) + w_2 f(b) + K f''(\xi), \quad \xi \in (a,b).$$

To find w_1 and w_2 we need to ensure that the formula is exact for all linear functions. However, using the principle of superposition, it is sufficient to make this work for any two independent linear polynomials (i.e. polynomials of degree one at most).
E.g. choose the two independent polynomials $f \equiv 1$ and $f \equiv x$.

$$\begin{aligned} \text{For } f \equiv 1 : \int_a^b \mathrm{d}x &= w_1 + w_2 = b - a; \\ \text{for } f \equiv x : \int_a^b x\,\mathrm{d}x &= a w_1 + b w_2 = \frac{b^2 - a^2}{2}. \end{aligned}$$

Solving these simultaneous equations gives

$$w_1 = w_2 = \frac{b-a}{2}.$$

To find the value of K, we can use any quadratic function so that $f''(\xi)$ is a non-zero constant, *independent* of the unknown ξ. E.g. take $f \equiv x^2$,

$$\begin{aligned} \int_a^b x^2\,\mathrm{d}x = \frac{b^3 - a^3}{3} &= \frac{b-a}{2}\left(a^2 + b^2\right) + 2K \quad (f'' = 2), \\ \Rightarrow 2K &= \frac{b^3 - a^3}{3} - \frac{b-a}{2}\left(a^2 + b^2\right), \\ &= (b-a)\left[\frac{1}{3}\left(a^2 + ab + b^2\right) - \frac{1}{2}\left(a^2 + b^2\right)\right], \\ &= (b-a)\left[-\frac{1}{6}\left(a^2 - 2ab + b^2\right)\right] = -\frac{(b-a)^3}{6}, \\ \Rightarrow K &= -\frac{(b-a)^3}{12}. \end{aligned}$$

Hence,

$$\int_a^b f(x)\,\mathrm{d}x = \frac{b-a}{2}\left(f(a) + f(b)\right) - \frac{(b-a)^3}{12} f''(\xi), \quad \xi \in (a,b), \tag{4.3}$$

in agreement with § 4.2.1 (but easier to derive).

Simpson's rule

Three points integration rule derived using the method of undetermined coefficients.
Suppose that we add a quadrature point at the middle of the interval $[a,b]$,

$$\int_a^b f(x)\,\mathrm{d}x \approx w_1 f(a) + w_2 f\left(\frac{a+b}{2}\right) + w_3 f(b).$$

To avoid algebra, substitute $x = \dfrac{a+b}{2} + u$ and define $h = \dfrac{b-a}{2}$ so that the integral becomes

$$\int_{-h}^{h} F(u)\,\mathrm{d}u \approx w_1 F(-h) + w_2 F(0) + w_3 F(h), \quad \text{with } F(u) = f(x).$$

Since we have three unknowns, we can make this formula exact for all quadratic functions; so, let us use, e.g., $F \equiv 1$, $F \equiv u$ and $F \equiv u^2$.

$$F \equiv 1 \Rightarrow \int_{-h}^{h} \mathrm{d}u = 2h = w_1 + w_2 + w_3;$$

$$F \equiv u \Rightarrow \int_{-h}^{h} u\,\mathrm{d}u = 0 = -hw_1 + hw_3 \Rightarrow w_1 = w_3;$$

$$F \equiv u^2 \Rightarrow \int_{-h}^{h} u^2\,\mathrm{d}u = \frac{2}{3}h^3 = h^2 w_1 + h^2 w_3 \Rightarrow w_1 = w_3 = \frac{h}{3};$$

$$w_2 = 2h - w_1 - w_3 = 2h - \frac{2}{3}h = \frac{4}{3}h.$$

Hence we obtain the approximation

$$\int_{-h}^{h} F(u)\,\mathrm{d}u \approx \frac{h}{3}F(-h) + \frac{4h}{3}F(0) + \frac{h}{3}F(h),$$

which translates into

$$\int_a^b f(x)\,\mathrm{d}x \approx \frac{b-a}{6}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right].$$

This is called Simpson's rule.

As this formula is exact for all quadratic functions, we expect the error to be of the form $KF'''(\xi)$.

However, if we examine $F \equiv u^3$, the integral $\int_{-h}^{h} u^3\,\mathrm{d}u = 0$ and Simpson's rule gives

$$\frac{h}{3}\left[(-h)^3 + 4 \times 0 + h^3\right] = 0 \Rightarrow K \equiv 0.$$

Therefore Simpson's rule is exact for cubic functions as well. Consequently, we try an error term of the form $KF^{(\mathrm{iv})}(\xi)$, $\xi \in (-h, h)$.

To find the value of K use, e.g., $F(u) \equiv x^4$ (with $F^{(\mathrm{iv})}(\xi) = 4!$, independent of ξ).

$$\int_{-h}^{h} u^4 \mathrm{d}u = \frac{2h^5}{5} = \frac{h}{3}\left[(-h)^4 + h^4\right] + 4!K \Rightarrow 4!K = 2h^5\left[\frac{1}{5} - \frac{1}{3}\right] = -\frac{4h^5}{15},$$

$$\Rightarrow K = -\frac{h^5}{90}.$$

Simpson's rule is fifth-order accurate: the error varies as the fifth power of the width of the interval.

Simpson's rule is given by

$$\int_a^b f(x)\,\mathrm{d}x = \frac{b-a}{6}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right] - \frac{(b-a)^5}{2880}\,f^{(\mathrm{iv})}(\xi), \quad \xi \in (a,b). \tag{4.4}$$

Example 4.1

Material covered in class. Please, see your lecture notes.

Closed Newton-Cotes formula of higher order can be derived using more equispaced intermediate points ($n = 2$: trapezium; $n = 3$: Simpson).

As observed for Simpson's rule, the error for n odd is of order $(b-a)^{n+2}$ rather than $(b-a)^{n+1}$, due to symmetry.

4.3 Open Newton-Cotes formulae

Closed Newton-Cotes formulae such as (4.3) and (4.4) include the value of the function at the endpoints.

By contrast, *open Newton-Cotes* formulae are based on the interior points only.

Midpoint rule. For example, consider the open Newton-Cotes formula

$$\int_a^b f(x)\,\mathrm{d}x \approx w_1 f\left(\frac{a+b}{2}\right).$$

Again, we can substitute $u = x - \dfrac{a+b}{2}$ and $h = \dfrac{b-a}{2}$;

$$\int_{-h}^{h} F(u)\,\mathrm{d}u \approx w_1 F(0).$$

This formula must hold for constant functions. So, taking, e.g. $F \equiv 1 \Rightarrow 2h = w_1$. However, since for $F(u) \equiv u$, $\displaystyle\int_{-h}^{h} F(u)\,\mathrm{d}u = 0$, the quadrature rule is exact for linear functions as well. So, we look for an error of the form $KF''(\xi)$, $\xi \in (-h, h)$;

$$\int_{-h}^{h} F(u)\,\mathrm{d}u = 2hF(0) + KF''(\xi), \quad \xi \in (-h, h).$$

Substitute $F(u) = u^2$,

$$\frac{2}{3}h^3 = 0 + 2K \Rightarrow K = \frac{h^3}{3}.$$

$$\int_a^b f(x)\,\mathrm{d}x = (b-a) f\left(\frac{a+b}{2}\right) + \frac{(b-a)^3}{24} f''(\xi), \quad \xi \in (a, b). \tag{4.5}$$

Same order as trapezium and coefficient of the error smaller (halved).

Example 4.2

Material covered in class. Please, see your lecture notes.

4.4 Gauss quadrature

There is no necessity to use equispaced points. By choosing the quadrature points x_k appropriately we can derive n-points methods of order $2n+1$ (i.e. error varies as $(b-a)^{2n+1}$), exact for polynomials of degree $(2n-1)$.

These are called *Gauss formulae* and can give stunning accuracy. However, for $n \geq 2$, the values of x_k (roots of Legendre polynomials) and the weights w_k are non rational.

4.5 Composite methods

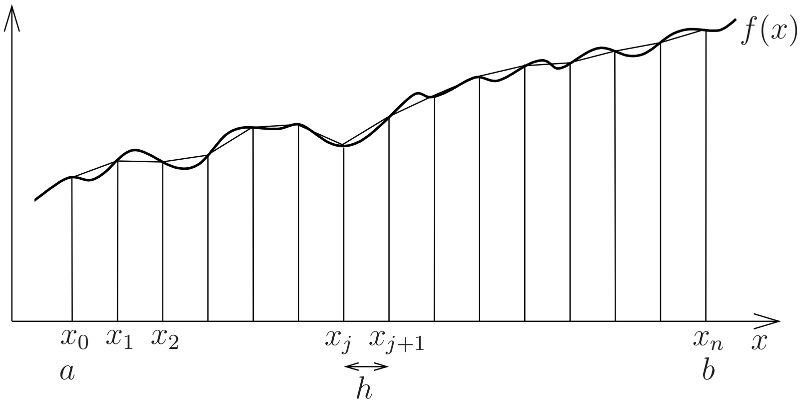
Disadvantage of higher order methods: Since higher order methods are based on Lagrange interpolation, they also suffer the same weaknesses.

While very accurate for functions with well-behaved higher order derivatives, they becomes inaccurate for functions with unbounded higher derivatives.

Therefore, it is often safer to use low order methods, such as trapezium and Simpson's rules. While these quadrature rules are not very accurate on large intervals (error varying as $(b-a)^3$ and as $(b-a)^5$), accurate approximations can be obtained by breaking the interval $[a,b]$ into n subintervals of equal width h.

4.5.1 Composite trapezium rule

Split the interval $[a,b]$ into n intervals of width $h = \dfrac{b-a}{n}$, i.e. consider $n+1$ equispaced points $x_j = a + jh$, $j = 0,\dots,n$. The subinterval j is $[x_j, x_{j+1}]$, $j = 0,\dots,n-1$.



$$\int_a^b f(x)\,\mathrm{d}x = \sum_{j=0}^{n-1}\int_{x_j}^{x_{j+1}} f(x)\,\mathrm{d}x = \sum_{j=0}^{n-1}\left\{\frac{h}{2}\left[f(x_j)+f(x_{j+1})\right] - \frac{h^3}{12}f''(\xi_j)\right\} \quad \xi_j \in (x_j, x_{j+1}),$$

$$\begin{aligned}\int_a^b f(x)\,\mathrm{d}x = \frac{h}{2}[f(a)+f(x_1)] + \frac{h}{2}[f(x_1)+f(x_2)] + \dots \\ + \frac{h}{2}[f(x_{n-2})+f(x_{n-1})] + \frac{h}{2}[f(x_{n-1})+f(b)] \\ - \frac{h^3}{12}\left[f''(\xi_0)+f''(\xi_1)+\dots+f''(\xi_{n-1})\right].\end{aligned}$$

<u>Error</u>: since

$$\min_j f''(\xi_j) \le K = \frac{1}{n}\sum_{j=0}^{n-1} f''(\xi_j) \le \max_j f''(\xi_j),$$

and f'' is continuous, there exits $\xi \in (a,b)$ with $f''(\xi) = K$ (analogous to the intermediate value theorem). Hence, the total error is of the form

$$E = -\frac{nh^3}{12}f''(\xi) = -\frac{b-a}{12}h^2 f''(\xi) \quad \text{since } b-a = nh.$$

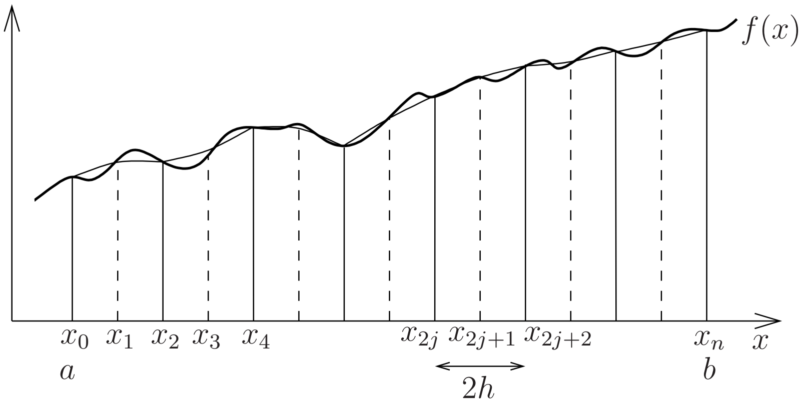
We can rewrite the composite trapezium rule as

$$\int_a^b f(x)\,\mathrm{d}x = \frac{h}{2}\left[f(a) + 2\sum_{j=1}^{n-1} f(x_j) + f(b)\right] - \frac{b-a}{12}h^2 f''(\xi), \quad \xi \in (a,b). \tag{4.6}$$

Composite trapezium rule has error of order h^2, compared to h^3 for each individual interval.

4.5.2 Composite Simpson's rule

Consider $n/2$ intervals $[x_{2j}, x_{2j+2}]$, $j = 0, \dots, n/2-1$, of width $2h = \dfrac{b-a}{n/2}$ with equispaced quadrature points $x_j = a + jh$, $j = 0, \dots, n$.



$$
\begin{aligned}
\int_a^b f(x)\,\mathrm{d}x &= \sum_{j=0}^{n/2-1} \int_{x_{2j}}^{x_{2j+2}} f(x)\,\mathrm{d}x, \\
&= \sum_{j=0}^{n/2-1} \left\{ \frac{h}{3}\left[f(x_{2j}) + 4f(x_{2j+1}) + f(x_{2j+2})\right] - \frac{h^5}{90} f^{(\mathrm{iv})}(\xi_j) \right\} \quad \xi_j \in [x_{2j}, x_{2j+2}],
\end{aligned}
$$

$$
\begin{aligned}
\int_a^b f(x)\,\mathrm{d}x = \frac{h}{3}[f(a) + 4f(x_1) + f(x_2)] + \frac{h}{3}[f(x_2) + 4f(x_3) + f(x_4)] + \dots \\
+ \frac{h}{3}[f(x_{n-2}) + 4f(x_{n-1}) + f(b)] - \frac{h^5}{90}\left[f^{(\mathrm{iv})}(\xi_0) + f^{(\mathrm{iv})}(\xi_1) + \dots + f^{(\mathrm{iv})}(\xi_{n/2-1})\right].
\end{aligned}
$$

As for the composite trapezium rule, there exists $\xi \in (a, b)$ such that

$$
\frac{n}{2} f^{(\mathrm{iv})}(\xi) = \sum_{j=0}^{n/2-1} f^{(\mathrm{iv})}(\xi_j).
$$

Using also $h = \dfrac{b-a}{n}$, we can rewrite the composite Simpson's rule as

$$
\begin{aligned}
\int_a^b f(x)\,\mathrm{d}x = \frac{h}{3}\left[f(a) + 2\sum_{j=1}^{n/2-1} f(x_{2j}) + 4\sum_{j=0}^{n/2-1} f(x_{2j+1}) + f(b)\right] \\
- \frac{b-a}{180} h^4 f^{(\mathrm{iv})}(\xi), \quad \xi \in (a, b). \quad (4.7)
\end{aligned}
$$

So, the composite Simpson's rule is 4^{th} order accurate.