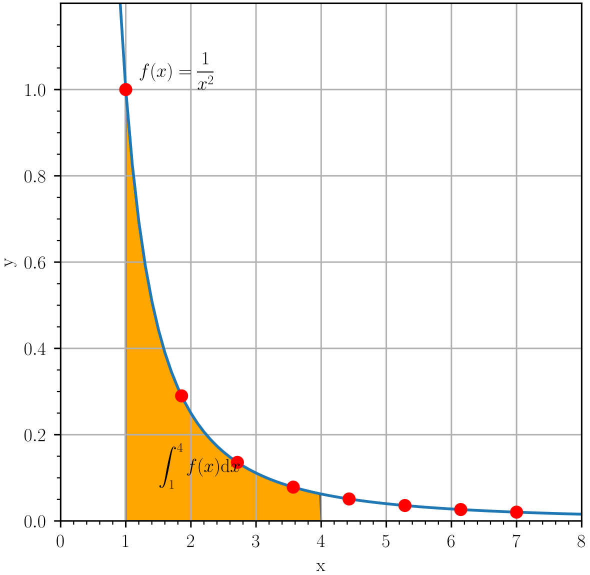
6. Integration

Integrals

Numerical methods can be used to find the value of definite integrals, if they can't be obtained analytically.
To estimate $I = \int_a^b f(x)dx$, numerical methods (*quadrature rules*) use the function value at different points between a and b. They can be thought of as trying to estimate the average value of f, which when multiplied by the interval length $(b-a)$ gives the integral.

Integral example



Trapezoid rule

$$I \approx T = (b - a)\frac{f(a) + f(b)}{2}$$

This estimates the average value of f using the values at the interval endpoints.

When the function second derivative is positive, $T > I$.

Midpoint rule

$$I \approx M = (b-a)f\left(\frac{a+b}{2}\right)$$

When the function second derivative is positive, $M < I$.

Simpson's rule

$$I \approx S = \frac{2}{3}M + \frac{1}{3}T = (b-a)\frac{f(a) + 4f(\frac{a+b}{2}) + f(b)}{6}$$

This has the right value when the function second derivative is constant; error is proportional to a higher derivative of f.

Composite rules

We can achieve better accuracy by dividing the interval $[a, b]$ into parts, applying a quadrature rule to each part separately, and summing the results.

For example, with the trapezoid rule and dividing $[a, b]$ into 4 equal-length intervals, we have

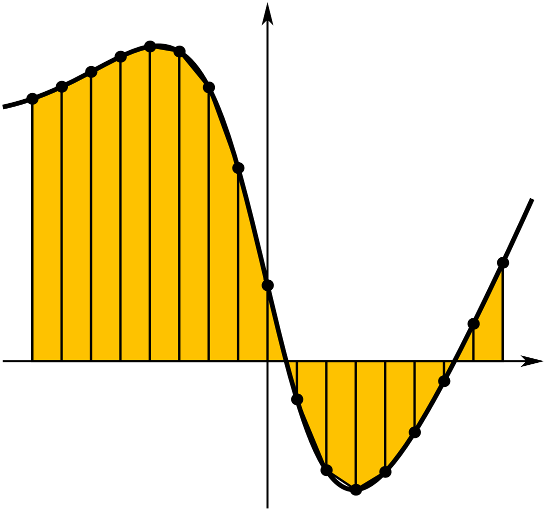
$$T_4 = w\frac{f(x_0) + f(x_1)}{2} + w\frac{f(x_1) + f(x_2)}{2} + w\frac{f(x_2) + f(x_3)}{2} + w\frac{f(x_3) + f(x_4)}{2}$$

$$= \frac{w}{2}(f(x_0) + 2[f(x_1) + f(x_2) + f(x_3)] + f(x_4))$$

where $w = \frac{b-a}{4}, x_0 = a, x_1 = a + \frac{b-a}{4}, x_2 = a + 2\frac{b-a}{4}, x_3 = a + 3\frac{b-a}{4}, x_4 = b$.

For equal spacing with general n, we can write $T_n = \frac{b-a}{2n}\left[f(a) + f(b) + 2\sum_{i=1}^{n-1} f(a + i\frac{b-a}{n})\right]$.

Composite trapezoid rule illustration



Remainder terms for composite quadrature rules

Assuming that f is sufficiently smooth,

$$R_T = -\frac{(b-a)^3}{12}\frac{f''(\xi)}{n^2}$$

$$R_M = \frac{(b-a)^3}{24}\frac{f''(\xi)}{n^2}$$

$$R_S = -\frac{(b-a)^5}{180}\frac{f^{(4)}(\xi)}{n^4}$$

with the derivatives evaluated in each case at some ξ between a and b

Combining different composite estimates to reduce truncation error

Similar to the centered finite difference approximation to the derivative, the trapezoid rule approximation to the integral has an error series that only has even powers of the subinterval width $h = \frac{(b-a)}{n}$.

If we had the trapezoid rule with N subintervals along with the more refined one with $2N$ subintervals, we can cancel out the error term proportional to h^2 with

$$\frac{4}{3} T_{2N} - \frac{1}{3} T_N.$$

In fact, this gives Simpson's rule with N subintervals, whose error is proportional to h^4.

We can repeat this process to then cancel out more terms $(h^4, h^6, \ldots)$, improving the accuracy for small enough h.

Romberg integration

This is systematized in an algorithm as follows:
Given a function f, where R_0^0 is the simple trapezoid rule estimate of the integral I of f between a and b:
Estimates with smaller step size are obtained as $R_i^0 = T_n$ (composite trapezoid rule) with $n = 2^i$
Combined estimates, which cancel out terms in the error series, are obtained as

$$R_i^j \equiv \frac{4^j}{4^j - 1} R_{i+1}^{j-1} - \frac{1}{4^j - 1} R_i^{j-1},$$

for $j = 1, 2, \ldots$

Example

For $f(x) = \sqrt{x}$, we can estimate the integral between 1 and 2 using Romberg integration via

$R_0^0 = \frac{\sqrt{1}+\sqrt{2}}{2} = 1.2071$

$R_1^0 = \frac{R_0^0}{2} + \frac{\sqrt{1.5}}{2} = 1.2159$

$R_0^1 = \frac{4}{3}R_1^0 - \frac{1}{3}R_0^0 = 1.21887$

$R_2^0 = \frac{R_1^0}{2} + \frac{\sqrt{1.25}+\sqrt{1.75}}{4} = 1.2182$

$R_1^1 = \frac{4}{3}R_2^0 - \frac{1}{3}R_1^0 = 1.218945$

$R_0^2 = \frac{16}{15}R_1^1 - \frac{1}{15}R_0^1 = 1.218950$

If we reached a certain maximum $j \geq 1$, we can estimate the absolute error in our highest-order estimate R_0^j using the difference between it and the second-best estimate: $|R_0^j - R_1^{j-1}|$

A graphical representation

ROMBERG INTEGRATION TABLE

$$
\begin{array}{cccccc}
n & T_0(n) & T_1(n) & T_2(n) & T_3(n) & T_4(n) \\
2 & T_0(2) & \to T_1(2) & T_2(2) & T_3(2) & T_4(2) \\
4 & T_0(4) & \to T_1(4) & T_2(4) & T_3(4) & \to T_4(4) \\
8 & T_0(8) & T_1(8) & T_2(8) & T_3(8) & \\
16 & T_0(16) & T_1(16) & \to T_2(16) & & \\
32 & T_0(32) & T_1(32) & & & \\
64 & T_0(64) & & & &
\end{array}
$$

$\theta(h^{2(4+1)})$

Gauss quadrature

This is another numerical integration approach. These quadrature rules use non equally spaced points that give the right value for integrals of functions that are as high degree polynomials as possible.

The general formula is $G_n = \sum_{i=1}^{n} w_i f(x_i)$ when integrating from -1 to 1 (where the w_i and x_i are given for any n)

And $G_n = \frac{b-a}{2} \sum_{i=1}^{n} w_i \cdot f\left(a + \frac{b-a}{2}(x_i + 1)\right)$ when integrating between any a and b

Thus, for $n = 2$, the points x_i are $-\frac{1}{\sqrt{3}}, +\frac{1}{\sqrt{3}}$ and the weights w_i are $1, 1$, so for the square root example $G_2 = 1.21901$

For $n = 3$, the points x_i are $-\sqrt{\frac{3}{5}}, 0, +\sqrt{\frac{3}{5}}$ and the weights w_i are $\frac{5}{9}, \frac{8}{9}, \frac{5}{9}$, so for the square root example $G_3 = 1.218952$