Numerical Methods
Differentiation and Integration

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Exact and numerical differentiation

Exact differentiation For most functions, the derivatives can be computed exactly using the formulae from Calculus.

e.g. $f(x) = x\sin(x) \implies f'(x) = x\cos(x) + \sin(x)$.

Numerical differentiation The aim of numerical differentiation is to estimate the derivatives $f'(x)$ of a function f at a point x for cases where exact computation is impossible or impractical, such as:

- The function is determined by experimentally-measured data i.e. $f(x_i) = y_i$.
- The function is determined by numerically-computed data e.g. the numerical solution of a differential equation.
- The function is specified by black-box code, and only supports the operation of evaluation at points.
- Explicitly computing the derivative would result in a formula which is too complicated to be efficiently stored and/or evaluated.

Numerical differentiation techniques

Finite-difference Compute approximations to derivatives using weighted sums/differences of function values.

Formulae are based on polynomial interpolation at nearby data points.

Automatic differentiation (Off-syllabus) A modern technique for computing derivatives exactly without constructing a symbolic formula explicitly.
Typically requires access to source code.

Finite-difference approximation

Derivative definition Recall from Calculus that:

$$f'(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h},$$

Difference approximation Estimate the derivative from the defining formula with $|h|$ small:

$$f'(x) \approx \frac{f(x+h) - f(x)}{h}$$

Note that h may be positive or negative!

Forward/backward difference

Example For $f(x) = 1/(1+x^2)$, estimate $f'(x)$ at $x = 2$ using the forward difference approximation with $h = 0.5, 0.1, 0.01, -0.1$.

$$f'(2) \approx \frac{f(2+0.5)-f(2)}{0.5} = \frac{\frac{1}{1+2.5^2} - \frac{1}{1+2^2}}{0.5} = \frac{\frac{1}{7.25} - \frac{1}{5}}{0.5} = \frac{0.138-0.200}{0.5} = -0.124$$

$$f'(2) \approx \frac{f(2+0.1)-f(2)}{0.1} = \frac{\frac{1}{1+2.1^2} - \frac{1}{1+2^2}}{0.1} = \frac{0.1848-0.2000}{0.1} = -0.1516$$

$$f'(2) \approx \frac{f(2+0.01)-f(2)}{0.01} = \frac{\frac{1}{1+2.01^2} - \frac{1}{1+2^2}}{0.01} = \frac{0.19841-0.20000}{0.01} = -0.15912$$

$$f'(2) \approx \frac{f(2-0.1)-f(2)}{-0.1} = \frac{\frac{1}{1+1.9^2} - \frac{1}{1+2^2}}{-0.1} = \frac{0.2169-0.2000}{-0.1} = -0.1692$$

Exact value

$$f'(x) = \frac{-2x}{(1+x^2)^2}; \quad f'(2) = \frac{-2 \times 2}{(1+2^2)^2} = \frac{-4}{25} = -0.1600.$$

Error is fairly large... What are the asymptotics for small h? Can we do better??

2-point forward difference

Forward difference error By Taylor's theorem, for some ξ between x and $x+h$,

$$f(x+h) = f(x) + hf'(x) + h^2 f''(\xi)/2.$$

Rearranging gives

$$f'(x) = \frac{f(x+h) - f(x)}{h} - \frac{h}{2} f''(\xi).$$

Error term

$$\left| f'(x) - \frac{f(x+h) - f(x)}{h} \right| = \frac{h}{2} \left| f''(\xi) \right|.$$

Note that Taylor's theorem gives no way of finding the point ξ. (If it did, we could compute the derivative exactly!)

However, the error term does show the error is $O(h)$.

Backward difference error For some ξ between $x - h$ and x,

$$f'(x) = \frac{f(x) - f(x-h)}{h} + \frac{h}{2} f''(\xi).$$

Centred difference

Centered difference by quadratic interpolation
Recall interpolation of f at $x-h, x, x+h$ by a quadratic polynomial:

$$\begin{aligned} p(y) = f(x) &+ \frac{f(x+h)-f(x-h)}{2h}(y-x) \\ &+ \frac{f(x-h)-2f(x)+f(x+h)}{2h^2}(y-x)^2. \end{aligned}$$

Compute the derivative:

$$\begin{aligned} p'(y) &= \frac{f(x+h)-f(x-h)}{2h} + \frac{f(x-h)-2f(x)+f(x+h)}{2h^2} \times 2(y-x); \\ p'(x) &= \frac{f(x+h)-f(x-h)}{2h}. \end{aligned}$$

Centred difference formula Estimate $f'(x)$ by $p'(x)$:

$$f'(x) \approx \frac{f(x+h)-f(x-h)}{2h}.$$

This is called the *three-point* centred difference formula, even though only two function values are needed! The formula is 'missing' the term $0 \times f(x)$.

Centred difference

Centred difference by Taylor series Combine forwards and backwards difference approximations:

$$\begin{aligned} f(x+h) &= f(x) + hf'(x) + h^2 f''(x)/2 + O(h^3) \\ f(x-h) &= f(x) - hf'(x) + h^2 f''(x)/2 + O(h^3) \end{aligned}$$

$$f(x+h) - f(x-h) = 2hf'(x) + O(h^3)$$

Hence

$$f'(x) = \frac{f(x+h)-f(x-h)}{2h} + O(h^2).$$

Centred difference formula

$$f'(x) \approx \frac{f(x+h)-f(x-h)}{2h}.$$

Centred difference error

Centered difference error estimate For some ξ between $x-h$ and $x+h$,

$$f'(x) = \frac{f(x+h)-f(x-h)}{2h} - \frac{h^2}{6} f'''(\xi).$$

Note method is exact for a quadratic polynomial!

Derivation by Taylor's theorem (Advanced)

$$\begin{aligned} f(x+h) &= f(x) + hf'(x) + h^2 f''(x)/2 + h^3 f'''(\xi_+)/6 \\ f(x-h) &= f(x) - hf'(x) + h^2 f''(x)/2 - h^3 f'''(\xi_-)/6 \end{aligned}$$

$$f(x+h) - f(x-h) = 2hf'(x) + h^3\big(f'''(\xi_+) + f'''(\xi_-)\big)/6$$

Since $\big(f'''(\xi_+) + f'''(\xi_-)\big)/2$ lies between $f'''(\xi_+)$ and $f'''(\xi_-)$, there exists ξ such that $f'''(\xi) = (f'''(\xi_+) + f'''(\xi_-)/2$, so

$$f(x+h) - f(x-h) = 2hf'(x) + h^3 f'''(\xi)/3.$$

Centred difference

Example Use the centred difference method with $h = 0.1, 0.01$ to estimate $f'(x)$ at $x = 2$.

$$f'(2) \approx \frac{f(2+0.1) - f(2-0.1)}{2 \times 0.1} = \frac{\frac{1}{1+(2+0.1)^2} - \frac{1}{1+(2-0.1)^2}}{2 \times 0.1} = \frac{\frac{1}{5.41} - \frac{1}{3.61}}{0.2}$$
$$= \big(0.18484 - 0.21792\big)/0.2 = -0.16039.$$

$$f'(2) \approx \frac{f(2+0.01) - f(2-0.01)}{2 \times 0.01} = \frac{\frac{1}{1+(2+0.01)^2} - \frac{1}{1+(2-0.01)^2}}{2 \times 0.1} = \frac{\frac{1}{5.0401} - \frac{1}{3.9601}}{0.02}$$
$$= \big(0.19840876 - 0.2016088\big)/0.02 = -0.1600038.$$

Centred difference

Error dependence Estimate $f'(2)$ by using the three-point centred-difference method with $h = 10^{-n}$ for $n = 0, \ldots, 14$.

h	f'	$\lvert e\rvert$
10^{-0}	-0.200000000000000	$0.040000000000000 \approx 4\times10^{-2}$
10^{-1}	-0.160384280736645	$0.000384280736645 \approx 4\times10^{-4}$
10^{-2}	-0.160003840028156	$0.000003840028156 \approx 4\times10^{-6}$
10^{-3}	-0.160000038399985	$0.000000038399985 \approx 4\times10^{-8}$
10^{-4}	-0.160000000384158	$0.000000000384158 \approx 4\times10^{-10}$
10^{-5}	-0.160000000004601	$0.000000000004601 \approx 5\times10^{-12}$
10^{-6}	-0.160000000012928	$0.000000000012928 \approx 1\times10^{-11}$
10^{-7}	-0.159999999915783	$0.000000000084217 \approx 8\times10^{-11}$
10^{-8}	-0.159999999360672	$0.000000000639328 \approx 6\times10^{-10}$
10^{-9}	-0.160000013238459	$0.000000013238459 \approx 1\times10^{-8}$
10^{-10}	-0.159999929971733	$0.000000070028267 \approx 7\times10^{-8}$
10^{-11}	-0.159999791193854	$0.000000208806146 \approx 2\times10^{-7}$
10^{-12}	-0.160024771211909	$0.000024771211908 \approx 2\times10^{-5}$
10^{-13}	-0.159872115546023	$0.000127884453977 \approx 1\times10^{-4}$
10^{-14}	-0.160982338570648	$0.000982338570648 \approx 1\times10^{-3}$

Small changes in computed $f(x\pm h)$ cause large change in derivative for small h!!

Truncation and roundoff error

Example For $f(x) = 1/(3+x^2)$, have $f'(x) = -2x/(3+x^2)^2$ and $f'''(x) = 24x(3-x^2)/(3+x^2)^4$, with $f'(2.0) = -0.081632\,(6\,\text{dp})$. Rounding to $3\,$dp gives

x	1.9	2.0	2.1
$y \approx f(x)$	0.151	0.143	0.135

Using the three-point centred-difference approximation to find $f'(2.0)$ yields $f'(2.0) \approx -0.08$, which has an absolute error of 1.63×10^{-3} $(2\,\text{sf})$.

Since for $\xi \in [1.9, 2.1]$, $-0.024 \le f'''(\xi) \le -0.014$ for all ξ, we can estimate the truncation error as

$$\sup_{\xi\in[1.9,2.1]}\lvert f'''(\xi)\rvert\frac{h^2}{6} \approx 0.024 \times \frac{0.1^2}{6} = 5\times10^{-5}.$$

The roundoff error is

$$\left\lvert\frac{f(x+h) - f(x-h)}{2h} - \frac{0.135 - 0.151}{2\times 0.1}\right\rvert \le 1.67\times10^{-3}.$$

Hence the main source of error is rounding in the y-values, and *not* the truncation error of the approximation.

Centred difference

Example Estimate $f'(x)$ for $x = 2.0, 2.2, 2.4, 2.6, 2.8, 3.0$ from the following data:

x	2.0	2.2	2.4	2.6	2.8	3.0
$f(x)$	1.386	1.735	2.101	2.484	2.883	3.296

$$f'(2.2) \approx (f(2.4) - f(2.0))/(2\times 0.2) = (2.101 - 1.386)/0.4 = 1.79$$

$$f'(2.4) \approx (f(2.6) - f(2.2))/(2\times 0.2) = (2.484 - 1.735)/0.4 = 1.87$$

$$f'(2.6) \approx (f(2.8) - f(2.4))/(2\times 0.2) = (2.883 - 2.101)/0.4 = 1.96$$

$$f'(2.8) \approx (f(3.0) - f(2.6))/(2\times 0.2) = (3.296 - 2.484)/0.4 = 2.03$$

Can't estimate $f'(2.0)$ and $f'(3.0)$ using centred difference!

Need a different formula for use at endpoints.

Forward/backward difference

Endpoints of domain For f defined on interval $[a, b]$, cannot use centred difference at/near endpoints a, b, as $f(a - h)$ and $f(b + h)$ are not defined!

Three-point forward-difference formula

$$f'(x) \approx \frac{-f(x + 2h) + 4f(x + h) - 3f(x)}{2h}.$$

Three-point forward-difference error estimate

$$f'(x) = \frac{-f(x + 2h) + 4f(x + h) - 3f(x)}{2h} + \frac{h^2}{3} f'''(\xi).$$

Three-point backward-difference Take h negative in forward-difference formula:

$$f'(x) \approx \frac{f(x - 2h) - 4f(x - h) + 3f(x)}{2h}.$$

Forward/backward difference

Example For $f(x) = 1/(1 + x^2)$, estimate $f'(2)$ using the forward-difference formula with $h = 0.1$.

$$f'(2) \approx \frac{-f(2 + 2\times 0.1) + 4f(2 + 0.1) - 3f(2)}{2h} = \frac{-f(2.2) + 4f(2.1) - 3f(2.0)}{2 \times 0.1}$$

$$= \frac{-0.171 + 4 \times 1.85 - 3 \times 2.00}{0.2} = -0.159307$$

Exact value -1.6; error 7.9×10^{-4}, roughly twice that for centred difference.

Forward/backward difference

Example Estimate $f'(x)$ for $x = 2.0, 2.2, 2.4, 2.6, 2.8, 3.0$ from the following data:

x	2.0	2.2	2.4	2.6	2.8	3.0
$f(x)$	1.386	1.735	2.101	2.484	2.883	3.296

Use centred-difference where possible:

$$\begin{aligned} f'(2.0) &\approx (-f(2.4) + 4f(2.2) - 3f(2.0))/(2\times 0.2) \\ &= (-2.101 + 4\times 1.735 - 3\times 1.386)/0.4 = 1.70 \end{aligned}$$

$$f'(2.2) \approx (f(2.4) - f(2.0))/(2\times 0.2) = (2.101 - 1.386)/0.4 = 1.79$$

$$f'(2.4) \approx (f(2.6) - f(2.2))/(2\times 0.2) = (2.484 - 1.735)/0.4 = 1.87$$

$$f'(2.6) \approx (f(2.8) - f(2.4))/(2\times 0.2) = (2.883 - 2.101)/0.4 = 1.96$$

$$f'(2.8) \approx (f(3.0) - f(2.6))/(2\times 0.2) = (3.296 - 2.484)/0.4 = 2.03$$

$$\begin{aligned} f'(3.0) &\approx (f(2.6) - 4f(2.8) + 3f(3.0))/(2\times 0.2) \\ &= (2.484 - 4\times 2.883 + 3\times 3.296)/0.4 = 2.10 \end{aligned}$$

Five-point centred difference

Five-point centred difference formula

$$f'(x) \approx \frac{f(x-2h) - 8f(x-h) + 8f(x+h) - f(x+2h)}{12h}$$

Five-point centred difference error estimate

$$f'(x) = \frac{f(x-2h) - 8f(x-h) + 8f(x+h) - f(x+2h)}{12h} + \frac{h^4}{30} f^{(5)}(\xi)$$

Example Estimate $f'(x)$ for $f(x) = 1/(1+x^2)$ with $x = 2$ and $h = 0.1$.

$$\begin{aligned} f'(2) &\approx \frac{f(1.8) - 8f(1.9) + 8f(2.1) - f(2.2)}{12 \times 0.1} \\ &= \frac{0.2358491 - 8\times 0.2169197 + 8\times 0.1848429 - 0.1712329}{1.2} \\ &= -0.1599989 \text{ (7dp)} \end{aligned}$$

Error 1.1×10^{-6}, much better than three-point error 3.9×10^{-4}.

Five-point difference formulae

Five-point forward difference

$$f'(x) = \frac{-25f(x) + 48f(x+h) - 36f(x+2h) + 16f(x+3h) - 3f(x+4h)}{12h} + \frac{h^4}{5}f^{(5)}(\xi)$$

Five-point assymmetric difference

$$f'(x) = \frac{-3f(x-h) - 10f(x) + 18f(x+h) - 6f(x+2h) + f(x+3h)}{12h} - \frac{h^4}{20}f^{(5)}(\xi)$$

Five-point centred difference

$$f'(x) = \frac{f(x-2h) - 8f(x-h) + 8f(x+h) - f(x+2h)}{12h} + \frac{h^4}{30}f^{(5)}(\xi)$$

Backward-difference formulae can be obtained by taking h negative.

Five-point difference

Example Estimate $f'(x)$ for $x = 2.0, 2.2, 2.4$ from the following data:

x	2.0	2.2	2.4	2.6	2.8	3.0
$f(x)$	1.386	1.735	2.101	2.484	2.883	3.296

Use five-point formulae:

$$\begin{aligned} f'(2.0) &\approx (-25f(2.0) + 48f(2.2) - 36f(2.4) + 16f(2.6) - 3f(2.8))/(12\times 0.2) \\ &= (-25\times 1.386 + 48\times 1.735 - 36\times 1.735 + 16\times 2.484 - 3\times 2.883)/2.4 \\ &= (-34.650 + 83.280 - 75.636 + 39.744 - 8.649)/2.4 \\ &= 4.089/2.4 = 1.704 \text{ (3dp)} \end{aligned}$$

$$\begin{aligned} f'(2.2) &\approx (-3f(2.0) - 10f(2.2) + 18f(2.4) - 6f(2.6) + f(2.8))/(12\times 0.2) \\ &= (-3\times 1.386 - 10\times 1.735 + 18\times 1.735 - 6\times 2.484 + 2.883)/2.4 \\ &= (-4.158 - 17.350 + 37.818 - 14.904 + 2.883)/2.4 \\ &= 4.289/2.4 = 1.787 \text{ (3dp)} \end{aligned}$$

$$\begin{aligned} f'(2.4) &\approx (f(2.0) - 8f(2.2) + 8f(2.6) - f(2.8))/(12\times 0.2) \\ &= (1.386 - 8\times 1.735 + 8\times 2.484 - 2.883)/2.4 \\ &= (1.386 - 13.880 + 19.872 - 2.883)/2.4 = 4.495/2.4 = 1.873 \text{ (3dp)} \end{aligned}$$

Second derivative

Second derivative by quadratic interpolation

$$p(y) = f(x) + \frac{f(x+h) - f(x-h)}{2h}(y-x) + \frac{f(x-h) - 2f(x) + f(x+h)}{2h^2}(y-x)^2.$$

Compute the derivatives:

$$p'(y) = \frac{f(x+h) - f(x-h)}{2h} + \frac{f(x-h) - 2f(x) + f(x+h)}{2h^2} \times 2(y-x);$$

$$p''(y) = \frac{f(x-h) - 2f(x) + f(x+h)}{2h^2} \times 2.$$

Three-point second-derivative formula Estimate $f''(x)$ by $p''(x)$:

$$f''(x) \approx \frac{f(x-h) - 2f(x) + f(x+h)}{h^2}.$$

Second derivative

Example For $f(x) = 1/(1+x^2)$, estimate $f''(2)$ using $h = 0.1, 0.01$.

$$f''(2) \approx \frac{f(2.1) - 2f(2) + f(1.9)}{0.1^2} = \frac{\frac{1}{5.41} - 2\times\frac{1}{5} + \frac{1}{4.61}}{0.01}$$

$$\approx \frac{0.184843 - 2 \times 0.200000 + 0.216920}{0.01} = \frac{0.001763}{0.01} = 0.1763\,.$$

$$f''(2) \approx \frac{f(2.01) - 2f(2) + f(1.99)}{0.01^2} = \frac{\frac{1}{5.0401} - 2\times\frac{1}{5} + \frac{1}{4.9601}}{0.0001}$$

$$\approx \frac{0.1984087617 - 2 \times 0.20000000 + 0.2016088385}{0.0001}$$

$$= \frac{0.0000176003}{0.0001} = 0.176003\,.$$

The exact value is $f''(2) = \frac{22}{125} = 0.176$.

Second derivative

Second derivative with error term

$$f''(x) = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} - f^{(4)}(\xi)\,h^2/12.$$

Second derivative by Taylor series (Non-examinable)

$$\begin{aligned} f(x+h) &= f(x) + hf'(x) + h^2 f''(x)/2 + h^3 f'''(x)/6 + \cdots \\ f(x-h) &= f(x) - hf'(x) + h^2 f''(x)/2 - h^3 f'''(x)/6 + \cdots \end{aligned}$$

$$f(x+h) + f(x-h) = 2f(x) + 2h^2 f''(x)/2 + 2h^4 f''''(x)/24 + O(h^5)$$

Hence

$$f(x+h) - 2f(x) + f(x-h) = 2h^2 f''(x)/2 + 2h^4 f''''(x)/24 + O(h^5).$$

Second derivative

Three-point schemes for second derivative

$$f''(x) = \frac{f(x-h) - 2f(x) + f(x+h)}{h^2} - \frac{1}{12}h^2 f^{(4)}(\xi)$$

$$f''(x) = \frac{f(x) - 2f(x+h) + f(x+2h)}{h^2} - hf^{(3)}(\xi)$$

Five-point schemes for second derivative

$$f''(x) = \frac{-f(x-2h) + 16f(x-h) - 30f(x) + 16f(x+h) - f(x+2h)}{12h^2} + \frac{1}{90}h^4 f^{(6)}(\xi)$$

$$f''(x) = \frac{11f(x-h) - 20f(x) + 6f(x+h) + 4f(x+2h) - f(x+3h)}{12h^2} + \frac{1}{12}h^3 f^{(5)}(\xi)$$

$$f''(x) = \frac{35f(x) - 104f(x+h) + 114f(x+2h) - 56f(x+3h) + 11f(x+4h)}{12h^2} - \frac{5}{6}h^3 f^{(5)}(\xi)$$

Note that the centred-difference approximations have a higher order!

Higher derivatives (Non-examinable)

Five-point schemes for third derivative

$$f'''(x) = \frac{-f(x-2h) + 2f(x-h) - 2f(x+h) + f(x+2h)}{2h^3} - \frac{1}{4}h^2 f^{(5)}(\xi)$$

$$f'''(x) = \frac{-3f(x-h) + 10f(x) - 12f(x+h) + 6f(x+2h) - f(x+3h)}{2h^3} + \frac{1}{4}h^2 f^{(5)}(\xi)$$

$$f'''(x) = \frac{-5f(x) + 18f(x+h) - 24f(x+2h) + 14f(x+3h) - 3f(x+4h)}{2h^3} + \frac{7}{4}h^2 f^{(5)}(\xi)$$

Five-point scheme for fourth derivative

$$f''''(x) = \frac{f(x-2h) - 4f(x-h) + 6f(x) - 4f(x+h) + f(x+2h)}{h^4} - \frac{1}{6}h^2 f^{(6)}(\xi)$$

Exercise

Exercise Estimate $f'(2)$, $f'(3)$ and $f''(3)$ for $f(x) = 1/x$ using

x	2.0	2.5	3.0	3.5	4.0
$f(x)$	0.500	0.400	0.333	0.286	0.250

Estimate the errors by $|f^{(n)}(\xi)| \leq n!/2^{n+1}$.

Appendix: Derivations and Error Estimates (Non-examinable)

Derivation of three-point schemes

Let $q(y)$ interpolate f at $x-h$, x and $x+h$. Then

$$q(y) = f(x) + \frac{f(x+h) - f(x-h)}{2h}(y-x) + \frac{f(x+h) - 2f(x) + f(x-h)}{2h^2}(y-x)^2$$

Approximate $f'(x) \approx q'(x)$ and $f''(x) \approx q''(x)$

$$f'(x) \approx \frac{f(x+h) - f(x-h)}{2h}; \quad f''(x) \approx \frac{f(x+h) - 2f(x) + f(x-h)}{h^2}.$$

and

$$\begin{aligned} f'(x+h) \approx q'(x+h) &= \frac{f(x+h) - f(x-h)}{2h} + \frac{f(x+h) - 2f(x) + f(x-h)}{h} \\ &= \frac{3f(x+h) - 4f(x) + f(x-h)}{2h} \\ f'(x) &\approx \frac{3f(x) - 4f(x-h) + f(x-2h)}{2h} = \frac{-3f(x) + 4f(x+h) - f(x+2h)}{2h} \end{aligned}$$

Derivation of three-point schemes

Let $q(y)$ be a quadratic polynomial

$$q(y) = a_0 + a_1(y-x) + a_2(y-x)^2; \quad q'(y) = a_1 + 2a_2(y-x).$$

If q interpolates f at $x-h$, x and $x+h$, then

$$\begin{aligned} f(x) &= q(x) = a_0; \\ f(x+h) &= q(x+h) = a_0 + a_1 h + a_2 h^2; \\ f(x+2h) &= q(x+2h) = a_0 + 2a_1 h + 4a_2 h^2. \end{aligned}$$

Eliminate a_2 and a_0 by

$$f(x+2h) - 4f(x+h) = -2a_1 h - 3a_0 = -2a_1 h - 3f(x)$$

Approximate

$$f'(x) \approx q'(x) = a_1 = \frac{-f(x+2h) + 4f(x+h) - 3f(x)}{2h}$$

Derivation of five-point scheme by standard basis

Let $q(y)$ be a quartic polynomial

$$q(y) = a_0 + a_1(y-x) + a_2(y-x)^2 + a_3(y-x)^3 + a_4(y-x)^4.$$

If q interpolates f at $x-2h$, $x-h$, x, $x+h$ and $x+2h$, then

$$\begin{aligned} f(x-2h) = q(x-2h) &= a_0 - 2a_1h + 4a_2h^2 - 8a_3h^3 + 16a_4h^4; \\ f(x-h) = q(x-h) &= a_0 - a_1h + a_2h^2 - a_3h^3 + a_4h^4; \\ f(x) = q(x) &= a_0; \\ f(x+h) = q(x+h) &= a_0 + a_1h + a_2h^2 + a_3h^3 + a_4h^4; \\ f(x+2h) = q(x+2h) &= a_0 + 2a_1h + 4a_2h^2 + 8a_3h^3 + 16a_4h^4. \end{aligned}$$

Eliminate a_0, a_2 and a_4 by

$$f(x+2h) - f(x-2h) = 4a_1h + 16a_3h^3; \quad f(x+h) - f(x-h) = 2a_1h + 2a_3h^3.$$

Eliminate a_3 by

$$\big(f(x+2h) - f(x-2h)\big) - 8\big(f(x+h) - f(x-h)\big) = -12a_1h.$$

Approximate

$$f'(x) \approx q'(x) = a_1 = \frac{f(x-2h) - 8f(x-h) + 8f(x+h) - f(x+2h)}{12h}$$

Derivation of five-point scheme by Lagrange basis

Let $x_i = ih$ for $i = -2, -1, 0, 1, 2$.
Let l_{-2} be the Lagrange basis polynomial

$$l_{-2}(y) = \frac{(y+h)y(y-h)(y-2h)}{24h^4} = \frac{y^4 - 2hy^3 - h^2y^2 + 2h^3y}{24h^4}$$

satisfying

$$l_{-2}(-2h) = 1, \ l_{-2}(-h) = l_{-2}(0) = l_{-2}(h) = l_{-2}(2h) = 0$$

Since the term in y has coefficient $2h^3/24h^4$, have $l'_{-2}(0) = 1/12h$.
Let l_{-1} be the Lagrange basis polynomial

$$l_{-1}(y) = \frac{(y+2h)y(y-h)(y-2h)}{-6h^4} = \frac{-y^4 + hy^3 + 4h^2y^2 - 4h^3y}{6h^4}$$

satisfying

$$l_{-1}(-h) = 1, \ l_{-1}(-2h) = l_{-1}(0) = l_{-1}(h) = l_{-1}(2h) = 0$$

Since the term in y has coefficient $-4h^3/6h^4$, have $l'_{-1}(0) = -8/12h$.
Similarly, $l'_0(0) = 0$, $l'_1(0) = 8/12h$ and $l'_2(0) = -1/12h$.

Derivation of five-point scheme by Lagrange basis

If q is a quartic interpolating y at x_{-2}, x_{-1}, x_0, x_1 and x_2, then

$$q(y) = f(x_{-2})l_{-2}(y) + f(x_{-1})l_{-1}(y) + f(x_0)l_0(y) + f(x_1)l_1(y) + f(x_2)l_2(y)$$

so

$$\begin{aligned} q'(0) &= f(x_{-2})l'_{-2}(0) + f(x_{-1})l'_{-1}(0) + f(x_0)l'_0(0) + f(x_1)l'_1(0) + f(x_2)l'_2(0) \\ &= \frac{f(x_{-2}) - 8f(x_{-1}) + 8f(x_1) - f(x_2)}{12h} \end{aligned}$$

Hence approximate

$$f'(0) \approx q'(0) = \frac{f(-2h) - 8f(-h) + 8f(h) - f(2h)}{12h}$$

By shifting the x-axis, find

$$f'(x) \approx \frac{f(x-2h) - 8f(x-h) + 8f(x+h) - f(x+2h)}{12h}$$

Error estimate for centred difference

Error estimate for centred difference Fix x, h. A polynomial p interpolating f at $x-h, x, x+h$ and also satisfying $p'(x) = f'(x)$ is given by

$$p(y) = f(x) + f'(x)(y-x) + \frac{f(x-h) - 2f(x) + f(x+h)}{2h^2}(y-x)^2 + \Big(\frac{f(x+h) - f(x-h)}{2h^3} - \frac{f'(x)}{h^2}\Big)(y-x)^3.$$

Let $g(y) = p(y) - f(y)$. By the interpolation conditions, $g(x) = g'(x) = g(x-h) = g(x+h) = 0$, so $g'''(\xi) = 0$ for some $\xi \in [x-h, x+h]$.

For this ξ, we have $p'''(\xi) = f'''(\xi)$, or

$$6\Big(\frac{f(x+h) - f(x-h)}{2h^3} - \frac{f'(x)}{h^2}\Big) = f'''(\xi).$$

Rearranging gives

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} - \frac{f'''(\xi)}{6}h^2.$$

Error estimate for centred difference

Error estimate for centred difference Fix x, h. A polynomial p interpolating f at $x-h, x, x+h$ is given by

$$p(y) = f(x) + \frac{f(x+h) - f(x-h)}{2h}(y-x) + \frac{f(x-h) - 2f(x) + f(x+h)}{2h^2}(y-x)^2.$$

Note that

$$p'(x) = \frac{f(x+h) - f(x-h)}{2h}$$

A cubic q satisfying $q(x-h) = q(x) = q(x+h) = 0$ and $q'(x) = 1$ is

$$q(y) = (y-x)(1 - (y-x)^2/h^2).$$

Let $E = f'(x) - p'(x)$, and Let $g(y) = p(y) + Eq(y) - f(y)$.

Then $g(x) = g(x-h) = g(x+h) = g'(x) = 0$, so $g'''(\xi) = 0$ for some $\xi \in [x-h, x+h]$.

For this ξ, we have $Eq'''(\xi) = f'''(\xi)$, or

$$-6/h^2 E = -\frac{6}{h^2}\Big(f'(x) - \frac{f(x+h) - f(x-h)}{2h}\Big) = f'''(\xi)$$

Rearranging gives

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} - \frac{f'''(\xi)}{6}h^2.$$

Error estimate guess using polynomial

Let

$$p(y) = \frac{(y+2h)(y+h)y(y-h)(y-2h)}{4h^4} = \frac{(y^2-4h^2)(y^2-h^2)y}{4h^4} = \frac{y^5-5h^2y^3+4h^4y}{4h^4}$$

Then $p(y)=0$ when $y=-2h,-h,0,h,2h,$ but $p'(0)=1$ and $p^{(5)}(y)=30/h^4$.
Hence the error in approximating $p'(0)$ by the five-point centered difference formula is $p^{(5)}(\xi)h^4/30$.
This error also holds for any non-polynomial:

$$f'(x) = \frac{f(x-2h)-8f(x-h)+8f(x+h)-f(x+2h)}{12h} + \frac{1}{30}f^{(5)}(\xi)h^4$$

Numerical Integration

Integration in Matlab

The Matlab command `integral(f,a,b)` computes the definite integral

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

Example Use Matlab to compute

$$\int_1^4 \frac{1}{1+x^2}\,dx$$

Solution

```
f=@(x)1./(1+x.^2); a=1; b=4;
I=integral(f,a,b)
```

or even

```
I=integral(@(x)1./(1+x.^2),1,4)
```

Matlab yields the answer 0.540419500270584.
This is equal to the exact answer $\operatorname{atan}(4) - \operatorname{atan}(1)$ to 15 dp.

Riemann sums

Partition Partition interval $[a, b]$ by $P = \{a = x_0 < x_1 < x_2 < \cdots < x_{n-1} < x_n = b\}$.

Define spacing $h_i = \Delta x_i = x_{i+1} - x_i$.
Maximum spacing $\|P\| = \max_{i=0,\ldots,n-1}(x_{i+1} - x_i)$.

Riemann sum Choose $c_i \in [x_i, x_{i+1}]$ for $i = 0, \ldots, n-1$. Approximate

$$\int_a^b f(x)\,dx \approx \sum_{i=0}^{n-1}(x_{i+1} - x_i)f(c_i)$$

Riemann integral Limit of Riemann sums as $\|P\| \to 0$.

Midpoint and Trapezoid Rules

Midpoint rule

Single interval Approximate f over the interval $[a, b]$ by the constant $f(c)$ where $c = (a + b)/2$.

Simple midpoint rule Then

$$\int_a^b f(x)\,dx \approx M(f, [a, b]) := \int_a^b f(c)\,dx = (b - a)f(c) = (b - a)\, f\big(\tfrac{a+b}{2}\big).$$

Example For $f(x) = x^4$ on $[0, 1]$,

$$\textstyle\int_0^1 f(x)\,dx \approx M(f, [0, 1]) = (1 - 0)f(\frac{0+1}{2}) = (1 - 0)f(\frac{1}{2}) = 1 \times \frac{1}{16} = 1/16.$$

The exact value is $\int_0^1 f(x)\,dx = 1/5$; relative error 69%!

Midpoint rule

Partition Divide $[a, b]$ into n subintervals with nodes $a = x_0 < x_1 < \cdots < x_n = b$.
Let $P = \{x_0, x_1, \ldots, x_n\}$ and $h_i = x_{i+1} - x_i$.

Composite midpoint rule

$$\int_a^b f(x)\,dx \approx M(f, P) := \sum_{i=0}^{n-1} (x_{i+1} - x_i)\, f\Big(\frac{x_i + x_{i+1}}{2}\Big).$$

Writing $x_{i+1/2} = (x_i + x_{i+1})/2$,

$$\int_a^b f(x)\,dx \approx M(f, P) := \sum_{i=0}^{n-1} (x_{i+1} - x_i) f\big(x_{i+1/2}\big).$$

Equally-spaced nodes If $h_i \equiv h = (b - a)/n$, then $x_i = a + hi$ and

$$\int_a^b f(x)\,dx \approx M_n(f, [a, b]) := \frac{b-a}{n} \sum_{i=0}^{n-1} f\Big(\frac{x_i + x_{i+1}}{2}\Big) = h \sum_{i=0}^{n-1} f\big(a + (i + \tfrac{1}{2})h\big).$$

Alternative indexing: $M_n(f, [a, b]) = h \sum_{i=1}^{n} f\big(a + (i - \frac{1}{2})h\big)$.

Midpoint rule

Example Use the midpoint rule with $P = \{1.0, 1.5, 2.0, 3.0, 3.5, 4.0\}$ to estimate $\int_a^b f(x)dx$ with $f(x) = 1/(1 + x^2)$, $a = 1$, $b = 4$.

Table of function values $f(x_{i+1/2})$ for $i = 0, \ldots, 4$:

$x_{i+1/2}$	1.25	1.75	2.5	3.25	3.75
$f(x_{i+1/2})$	0.39024	0.24615	0.13793	0.08649	0.06639

Approximation

$$\begin{aligned} M(f, P) &= (x_1 - x_0) f(x_{\frac{1}{2}}) + (x_2 - x_1) f(x_{1\frac{1}{2}}) + (x_3 - x_2) f(x_{2\frac{1}{2}}) \\ &\qquad + (x_4 - x_3) f(x_{3\frac{1}{2}}) + (x_5 - x_4) f(x_{4\frac{1}{2}}) \\ &= (1.5 - 1.0) f(1.25) + (2.0 - 1.5) f(1.75) + (3.0 - 2.0) f(2.5) \\ &\qquad + (3.5 - 3.0) f(3.25) + (4.0 - 3.5) f(3.75) \\ &= 0.5 \times 0.39024 + 0.5 \times 0.24615 + 1.0 \times 0.13793 + 0.5 \times 0.08649 + 0.5 \times 0.06639 \\ &= 0.19512 + 0.12308 + 0.13793 + 0.04324 + 0.03320 = 0.53257 \text{ (5dp)} \end{aligned}$$

Exact answer $0.54041950 \cdots$, error 7.9×10^{-3}, relative error 1.5%.

Midpoint rule error analysis (non-examinable)

Error analysis For interval $[-h/2, +h/2]$, let $E = \int_{-h/2}^{h/2} f(x)dx - hf(0)$. Let

$$p(x) = f(0) + xf'(0) + 12Ex^2/h^3, \quad g(x) = p(x) - f(x).$$

Clearly

$$g(0) = 0 \quad \text{and} \quad g'(0) = 0.$$

Note that

$$\int_{-h/2}^{h/2} dx = h, \quad \int_{-h/2}^{h/2} x\,dx = 0 \text{ and } \int_{-h/2}^{h/2} x^2 dx = h^3/12.$$

Hence

$$\int_{-h/2}^{h/2} p(x)dx = hf(0) + 12E/h^3 \times h^3/12 = hf(0) + E = \int_{-h/2}^{h/2} f(x)dx.$$

Therefore $\int_{-h/2}^{h/2} g(x) = 0$, so g has a zero s in $(-h/2, h/2)$.

If the only zero of g is at 0, then $g''(0) = 0$ since g must change sign somewhere, and $g'(0) = 0$. If $s \neq 0$, then by Rolle's theorem, g' has a zero between s and 0, so g'' has a zero at $\xi \in (-h/2, h/2)$.

$$g''(\xi) = 24E/h^3 - f''(\xi) = 0 \implies E = h^3 f''(\xi)/24.$$

Midpoint rule error

Error term For the simple midpoint rule, there exists $\xi \in [a, b]$ such that

$$\int_a^b f(x)\,dx = (b-a)f\left(\tfrac{a+b}{2}\right) + \tfrac{1}{24} f''(\xi)(b-a)^3.$$

For the composite midpoint rule with n equal subdivisions of width h, there exists $\xi \in [a, b]$ such that

$$\int_a^b f(x)\,dx = \frac{b-a}{n} \sum_{i=0}^{n-1} f(x_{i+1/2}) + \frac{b-a}{24}\, h^2 f''(\xi).$$

Midpoint rule error bound (Advanced)

Norm of a partition For a partition P recall $||P|| := \sup_{i=1,\ldots,n}(x_i - x_{i-1})$.

Error bounds An upper bound for the error of the midpoint rule is

$$\left| \int_a^b f(x)dx - M(f, P) \right| \leq \frac{b-a}{24}\, ||P||^2 \sup_{\xi \in [a,b]} |f''(\xi)|.$$

For a partition into n equal subintervals of $[a, b]$ with width h, then

$$\left| \int_a^b f(x)dx - M_n(f, [a, b]) \right| \leq \frac{b-a}{24}\, h^2 \sup_{\xi \in [a,b]} |f''(\xi)|.$$

Suppose B_2 is a constant such that

$$\forall \xi \in [a, b],\ |f''(\xi)| \leq B_2.$$

Then for $||P|| \leq h$, an upper bound for the error is

$$\left| \int_a^b f(x)dx - M(f, P) \right| \leq \frac{b-a}{24}\, h^2\, B_2.$$

Midpoint rule error bound (Advanced)

Example How many subdivisions suffice to evaluate $\int_0^1 x^2\,dx$ to an accuracy of $\epsilon = 10^{-3}$ using the midpoint rule?

Note that $|f''(\xi)| = 2$ for all $\xi \in [0,1]$, so $B_2 := \sup_{\xi\in[0,1]} |f''(\xi)| = 2$.

For an error bound of at most ϵ, need

$$\frac{(b-a)^3 B_2}{24n^2} \le \epsilon.$$

Hence

$$n^2 \ge \frac{(b-a)^3 B_2}{24\epsilon} = \frac{1^3 \times 2}{24 \times 10^{-3}} = 10^3/12 = 83.\dot{3}$$

so require $n = 10$ with step-size $h = 0.1$.

Trapezoid rule

Single interval Interpolate f by a linear function l between a and b, so

$$l(x) = f(a) + \frac{x-a}{b-a}(f(b) - f(a)).$$

Note

$$\int_a^b \frac{x-a}{b-a}dx = \left[\frac{(x-a)^2}{2(b-a)}\right]_a^b = \frac{(b-a)^2}{2(b-a)} = \frac{b-a}{2}.$$

Hence

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

This is the area of the trapezoid with vertices $\{(a,0),(b,0),(a,f(a)),(b,f(b))\}$!

Simple trapezoid rule

$$\int_a^b f(x)\,dx \approx T(f,[a,b]) := (b-a)\frac{f(a)+f(b)}{2}$$

Example For $f(x) = x^4$ on $[0,1]$,

$$1/5 = \int_0^1 f(x)\,dx \approx T(f,[0,1]) = (f(0)+f(1))/2 = (0+1)/2 = 1/2.$$

Trapezoid rule

Composite trapezoid rule For partition $P = \{x_0, x_1, \ldots, x_n\}$, approximate the integral on each subinterval by the simple trapezoid rule:

$$\int_a^b f(x)\,dx \approx T(f,P) := \sum_{i=0}^{n-1}(x_{i+1}-x_i)\frac{f(x_i)+f(x_{i+1})}{2}.$$

Equally-spaced nodes With $h_i \equiv h = (b-a)/n$ and $x_i = a + hi$,

$$\int_a^b f(x)\,dx \approx T_n(f,[a,b]) := \frac{b-a}{n}\Big(\tfrac{1}{2}f(x_0) + \sum_{i=1}^{n-1} f(x_i) + \tfrac{1}{2}f(x_n)\Big)$$
$$= h\Big(\tfrac{1}{2}f(a) + \sum_{i=1}^{n-1} f(a+hi) + \tfrac{1}{2}f(b)\Big)$$

Trapezoid rule

Example Use the trapezoid rule with $n = 6$ to estimate

$$\int_1^4 \frac{1}{1+x^2}\,dx$$

Have $a = 1$, $b = 4$, $h = (b-a)/n = (4-1)/6 = 0.5$, $x_i = 1.0 + 0.5i$.
Table of function values $f(x) = 1/(1+x^2)$:

x_i	1.0	1.5	2.0	2.5	3.0	3.5	4.0
$f(x_i)$	0.50000	0.30769	0.20000	0.13793	0.10000	0.07547	0.05882

Approximation

$$\begin{aligned} T_6(f,[1,4]) &= h\big(\tfrac{1}{2}f(x_0) + f(x_1) + f(x_2) + f(x_3) + f(x_4) + f(x_5) + \tfrac{1}{2}f(x_6)\big) \\ &= 0.5 \times \big(\tfrac{1}{2}\times 0.50000 + 0.30769 + 0.20000 + 0.13793 \\ &\qquad + 0.10000 + 0.07547 + \tfrac{1}{2}\times 0.05882\big) \\ &= \tfrac{1}{2}\big(0.25000 + 1.23077 + 0.40000 + 0.55172 + 0.20000 + 0.30189 + 0.02941\big) \\ &= \tfrac{1}{2}\times 1.10051 = 0.55025 \text{ (5dp)} \end{aligned}$$

Exact answer $0.54041950\cdots$, error 9.8×10^{-3}, relative error 1.8%.

Trapezoid rule error analysis (Non-examinable)

Error analysis For a single interval $[0,h]$, set $E = \int_0^h f(x)\,dx - h\frac{f(0)+f(h)}{2}$. Note

$$\int_0^h x(h-x)dx = [hx^2/2 - x^3/3]_0^h = h^3/2 - h^3/3 = h^3/6.$$

Let

$$g(x) = f(0) + x\frac{f(h)-f(0)}{h} + 6Ex(h-x)/h^3 - f(x).$$

Then

$$\int_0^h g(x)\,dx = hf(0) + \frac{h^2}{2h}\big(f(h) - f(0)\big) + E - \int_0^h f(x)\,dx = 0.$$

By the mean value theorem, there exists $s \in (0,h)$ such that $g(s) = 0$. Then g has roots $0, s, h$ in $[0,h]$. By Rolle's theorem, g' has two distinct roots in $(0,h)$, and g'' has a root ξ in $(0,h)$. Hence

$$g''(\xi) = -12E/h^3 - f''(\xi) = 0$$

So

$$E = \int_0^h f(x)\,dx - h\frac{f(0)+f(h)}{2} = -f''(\xi)h^3/12$$

Trapezoid rule error

Error term For the simple trapezoid rule, there exists $\xi \in [a,b]$ such that

$$\int_a^b f(x)\,dx = (b-a)\,\frac{f(a)+f(b)}{2} - \frac{1}{12}f''(\xi)(b-a)^3.$$

For the composite trapezoid rule with n equal subdivisions of width h, there exists $\xi \in [a,b]$ such that

$$\int_a^b f(x)\,dx = T_n(f,[a,b]) - \frac{b-a}{12}\,h^2 f''(\xi).$$

Trapezoid rule error bound (Advanced)

Error bound An upper bound for the error of the trapezoid rule is

$$\left|\int_a^b f(x)dx - T(f,P)\right| \le \frac{b-a}{12}\,||P||^2 \sup_{\xi\in[a,b]} |f''(\xi)|.$$

For a partition into n equal subintervals of $[a,b]$ with width h, then

$$\left|\int_a^b f(x)dx - T_n(f,[a,b])\right| \le \frac{b-a}{12}\,h^2 \sup_{\xi\in[a,b]} |f''(\xi)|.$$

Example For $f(x) = 1/(1+x^2)$, $a = 1$, $b = 4$, find $f''(x) = 2(4x^2-1)/(1+x^2)^3$ and $\sup_{\xi\in[1,4]} |f''(\xi)| = |f''(1)| = 0.75$.

So for $n = 6$, have $h = 0.5$ and error bound

$$E \le \tfrac{(b-a)}{12}\,h^2 \sup_{\xi\in[a,b]}|f''(\xi)| = \tfrac{4-1}{12} \times 0.5^2 \times 0.75 = \tfrac{3}{64} = 4.7\times 10^{-2} \text{ (2sf)}.$$

The actual error is 9.8×10^{-3}, well below the error bound.

Simpson's Rule

Simpson's rule

Single scaled interval Interpolate f by a quadratic polynomial at $-h, 0, h$.

$$p(x) = f(0) + \frac{f(h)-f(-h)}{2}\frac{x}{h} + \frac{f(h)-2f(0)+f(-h)}{2}\frac{x^2}{h^2}$$

Then

$$\begin{aligned}
\int_{-h}^{h} p(x)\,dx &= \int_{-h}^{h} f(0) + \frac{f(h)-f(-h)}{2}\frac{x}{h} + \frac{f(h)-2f(0)+f(-h)}{2}\frac{x^2}{h^2}\,dx \\
&= 2\int_0^h f(0) + \frac{f(h)-2f(0)+f(-h)}{2}\frac{x^2}{h^2}\,dx \\
&= 2\left[xf(0) + \frac{f(h)-2f(0)+f(-h)}{2}\frac{x^3}{3h^2}\right]_0^h \\
&= 2\Big(hf(0) + \frac{f(h)-2f(0)+f(-h)}{2}\frac{h^3}{3h^2}\Big) \\
&= \frac{2h}{6}\big(f(-h) + 4f(0) + f(h)\big)
\end{aligned}$$

Simpson's rule

Simple Simpson's rule

$$\int_a^b f(x)\,dx \approx S(f,[a,b]) = \frac{b-a}{6}\big(f(a) + 4f(\tfrac{a+b}{2}) + f(b)\big).$$

Error term

$$\int_a^b f(x)\,dx = \frac{b-a}{6}\big(f(a) + 4f(\tfrac{a+b}{2}) + f(b)\big) - \frac{f^{(4)}(\xi)}{2880}(b-a)^5.$$

Simpson's rule

Composite Simpson's rule; equally-spaced nodes For $n = 2m$ (even!) subintervals of length $h = (b-a)/n$ with $x_i = a + ih$:

$$\begin{aligned} S_n(f,[a,b]) &= \frac{h}{3}\big(f(x_0) + 4f(x_1) + 2f(x_2) + 4f(x_3) \\ &\qquad + 2f(x_4) + \cdots + 2f(x_{n-2}) + 4f(x_{n-1}) + f(x_n)\big) \\ &= \frac{h}{3}\Big(f(x_0) + 4\sum_{i=1}^{n/2} f(x_{2i-1}) + 2\sum_{i=1}^{n/2-1} f(x_{2i}) + f(x_n)\Big) \end{aligned}$$

Error bound A bound for the error on subdividing $[a,b]$ into $n = 2m$ subintervals of length $h = (b-a)/n$ is

$$\big|\int_a^b f(x)\,dx - S_n(f,[a,b])\big| \le \frac{(b-a)}{180}\,h^4 \sup_{\xi\in[a,b]} |f^{(4)}(\xi)|$$

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Simpson's rule

Simpson's rule, non-equal subdivisions For partition $P = a = x_0 < x_1 < \cdots < x_m = b$, set $x_{i+1/2} = (x_i + x_{i+1})/2$.

$$S(f,P) = \sum_{i=0}^{m-1} (x_{i+1} - x_i)\,\frac{f(x_i) + 4f(x_{i+1/2}) + f(x_{i+1})}{6}$$

Note that here we are evaluating f at points indexed

$$x_0, x_{\frac{1}{2}}, x_1, x_{1\frac{1}{2}}, x_2, \ldots, x_{m-1}, x_{m-\frac{1}{2}}, x_m!$$

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Simpson's rule

Polynomials For the third-order polynomial x^3, Simpson's rule is exact.

$$\int_{-h}^{h} x^3\,dx = 0; \quad S(x^3,[-h,+h]) = h((-h)^3 + h^3)/3 = 0.$$

For the fourth-order polynomial x^4, the error E of using Simpson's rule is

$$\int_{-h}^{h} x^4\,dx = 2h^5/5; \quad S(x^4,[-h,+h]) = 2h^5/3; \quad E = 4h^5/15$$

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Simpson's rule

Example Use Simpson's rule with $n = 6$ to estimate

$$\int_1^4 \frac{1}{1+x^2}\,dx$$

Have $a = 1$, $b = 4$, $h = (b-a)/n = (4-1)/6 = 0.5$, $x_i = 1.0 + 0.5i$.
Table of function values $f(x) = 1/(1+x^2)$:

x_i	1.0	1.5	2.0	2.5	3.0	3.5	4.0
$f(x_i)$	0.50000	0.30769	0.20000	0.13793	0.10000	0.07547	0.05882

Approximation

$$\begin{aligned} S_6(f,[1,4]) &= \frac{h}{3}\big(f(x_0)+4f(x_1)+2f(x_2)+4f(x_3)+2f(x_4)+4f(x_5)+f(x_6)\big) \\ &= \frac{0.5}{3}\big(0.50000+4\times 0.30769+2\times 0.20000+4\times 0.13793 \\ &\qquad +2\times 0.10000+4\times 0.07547+0.05882\big) \\ &= \tfrac{1}{6}\big(0.50000+1.23077+0.40000+0.55172+0.20000+0.30189+0.05882\big) \\ &= \tfrac{1}{6}\times 3.24320 = 0.54053 \text{ (5dp)} \end{aligned}$$

Exact answer $0.54041950\cdots$, error 1.1×10^{-4}, relative error 0.02%.

Newton-Cotes formulae

Simpson's three-eighths rule

$$\begin{aligned} \int_a^b f(x)\,dx &= \frac{b-a}{8}\big(f(a)+3f(\tfrac{2a+b}{3})+3f(\tfrac{a+2b}{3})+f(b)\big) - \frac{(b-a)^5}{6480}f^{(4)}(\xi) \\ &= \frac{3h}{8}\big(f(x_0)+3f(x_1)+3f(x_2)+f(x_3)\big) - \frac{(b-a)}{80}h^4 f^{(4)}(\xi). \end{aligned}$$

where $h = (b-a)/3$, $x_i = a + ih$.

Note that this formula uses three partition intervals, and has error $O(h^4)$, so can be used to apply Simpson's rule to the case of an odd number of partition intervals!

Sixth-order Newton-Cotes (Non-examinable)

$$\begin{aligned} \int_a^b f(x)\,dx &\approx \frac{b-a}{90}\big(7f(a)+32f(\tfrac{3a+b}{4})+12f(\tfrac{a+b}{2})+32f(\tfrac{a+3b}{4})+7f(b)\big) \\ &= \frac{2h}{45}\big(7f(x_0)+32f(x_1)+12f(x_2)+32f(x_3)+7f(x_4)\big) - \frac{2(b-a)}{945}h^6 f^{(6)}(\xi). \end{aligned}$$

where $h = (b-a)/4$, $x_i = a + ih$.

Gaussian quadrature (Non-examinable)

Two-point Gaussian quadrature

$$\begin{aligned}\int_{-1}^{+1} f(x)\,dx &= \big(f(-\sqrt{1/3}) + f(+\sqrt{1/3})\big) + \frac{b-a}{4320}h^4 f^{(4)}(\xi)\\ &\approx f(-0.57735027) + f(+0.57735027)\end{aligned}$$

where $b-a=h=2$.

Three-point Gaussian quadrature

$$\begin{aligned}\int_{-1}^{+1} f(x)\,dx &= \big(\tfrac{5}{9}f(-\sqrt{3/5}) + \tfrac{8}{9}f(0) + \tfrac{5}{9}f(+\sqrt{3/5})\big) + \frac{b-a}{2016000}h^6 f^{(6)}(\xi)\\ &\approx 0.55555556f(-0.77459667) + 0.88888889f(0.00000000)\\ &\quad + 0.55555556f(+0.77459667)\end{aligned}$$

Four-point Gaussian quadrature

$$\begin{aligned}\int_{-1}^{+1} f(x)\,dx &\approx 0.34785485f(-0.86113631) + 0.65214515f(-0.33998104)\\ &\quad + 0.65214515f(+0.33998104) + 0.34785485f(+0.86113631)\big)\end{aligned}$$

Romburg Integration

Richardson extrapolation

Richardson extrapolation Since the error of the trapezoid rule is $O(h^2)$, over a fixed interval $[a,b]$ we can estimate for $I(f) = \int_a^b f(x)dx$:

$$E_{T_{2n}} = I(f) - T_{2n}(f) \approx \tfrac{1}{4}(I(f) - T_n(f)) = \tfrac{1}{4}E_{T_n}.$$

Rearranging gives

$$T_{2n}(f) + E_{T_2} = I(f) \approx T_n(f) + 4E_{T_2} \implies E_{T_2} = \tfrac{1}{3}\big(T_{2n}(f) - T_n(f)\big)$$

so

$$\begin{aligned}I(f) &\approx T_{2n}(f) + \tfrac{1}{3}\big(T_{2n}(f) - T_n(f)\big)\\ &= \tfrac{1}{3}\big(4T_{2n}(f) - T_n(f)\big) = \tfrac{4}{3}T_{2n}(f) - \tfrac{1}{3}T_n(f).\end{aligned}$$

This gives an improved estimate of the integral!

For the case $n=1$,

$$\begin{aligned}\tfrac{4}{3}T_2(f) - \tfrac{1}{3}T_1(f) &= \tfrac{4}{3}\tfrac{b-a}{2}\big(\tfrac{1}{2}f(a) + f(\tfrac{a+b}{2}) + \tfrac{1}{2}f(b)\big) - \tfrac{1}{3}\tfrac{b-a}{1}\big(\tfrac{1}{2}f(a) + \tfrac{1}{2}f(b)\big)\\ &= \frac{b-a}{6}\big(f(a) + 4f(\tfrac{a+b}{2}) + f(b)\big).\end{aligned}$$

This is just Simpson's rule!

Richardson extrapolation

Richardson extrapolation of Simpson's rule Since the error of Simpson's rule is $O(h^4)$, we can estimate

$$S_{2n}(f) - I(f) \approx \tfrac{1}{16}(S_n(f) - I(f))$$

Rearranging gives

$$\begin{aligned} I(f) &\approx S_{2n}(f) + \tfrac{1}{15}\big(S_{2n}(f) - S_n(f)\big) \\ &= \tfrac{1}{15}\big(16S_{2n}(f) - S_n(f)\big) = \tfrac{16}{15}S_{2n}(f) - \tfrac{1}{15}S_n(f)\big). \end{aligned}$$

This gives a further improved estimate of the integral!

This idea of using two approximations of the same order, and attempting to cancel the errors is known as *Richardson extrapolation*.

For integration, this can be continued indefinitely, yielding *Romburg integration*.

Romburg integration

Romburg integration For fixed n, let $h_n = \frac{b-a}{n}$ and T_n the trapezoid approximation

$$T_n(f,[a,b]) = h_n\big(\tfrac{1}{2}f(a) + \textstyle\sum_{k=1}^{n-1} f(a+kh_n) + \tfrac{1}{2}f(b)\big).$$

Notice that we can reuse results of $f(\cdot)$ for $T_{2^{i-1}}$ in computing T_{2^i} since

$$T_{2m} = \tfrac{1}{2}T_m + h_{2m}\textstyle\sum_{k=1}^{m} f(a+(k-\tfrac{1}{2})h_m).$$

Define initial Romburg estimates

$$R_{i,0} = T_{2^i}$$

Apply Richardson extrapolation to obtain higher-order estimates for $j > 0$:

$$\begin{aligned} R_{i,j} &= R_{i,j-1} + \frac{R_{i,j-1} - R_{i-1,j-1}}{4^j - 1} \\ &= \frac{4^j\,R_{i,j-1} - R_{i-1,j-1}}{4^j - 1} \\ &= \frac{4^j}{4^j - 1}R_{i,j-1} - \frac{1}{4^j - 1}R_{i-1,j-1} \end{aligned}$$

Romburg integration

Write as a table

$R_{0,0} = T_1$			
$R_{1,0} = T_2$	$R_{1,1} = \frac{4}{3}R_{1,0} - \frac{1}{3}R_{0,0}$		
$R_{2,0} = T_4$	$R_{2,1} = \frac{4}{3}R_{2,0} - \frac{1}{3}R_{1,0}$	$R_{2,2} = \frac{16}{15}R_{2,1} - \frac{1}{15}R_{1,1}$	
$R_{3,0} = T_8$	$R_{3,1} = \frac{4}{3}R_{3,0} - \frac{1}{3}R_{2,0}$	$R_{3,2} = \frac{16}{15}R_{3,1} - \frac{1}{15}R_{2,1}$	$R_{3,3} = \frac{64}{63}R_{3,2} - \frac{1}{63}R_{2,2}$

Alternatively, use the formulae

$R_{0,0} = T_1$			
$R_{1,0} = T_2$	$R_{1,1} = \frac{1}{3}(4R_{1,0} - R_{0,0})$		
$R_{2,0} = T_4$	$R_{2,1} = \frac{1}{3}(4R_{2,0} - R_{1,0})$	$R_{2,2} = \frac{1}{15}(16R_{2,1} - R_{1,1})$	
$R_{3,0} = T_8$	$R_{3,1} = \frac{1}{3}(4R_{3,0} - R_{2,0})$	$R_{3,2} = \frac{1}{15}(16R_{3,1} - R_{2,1})$	$R_{3,3} = \frac{1}{63}(64R_{3,2} - R_{2,2})$

Romburg integration

Example Estimate $\int_0^\pi \sin x \, dx$ using Romburg integration computing $R_{3,3}$.

$$f(0) = f(\pi) = 0.000000; \quad f(\tfrac{\pi}{2}) = 1.000000; \quad f(\tfrac{\pi}{4}) = f(\tfrac{3\pi}{4}) = 0.707107;$$
$$f(\tfrac{\pi}{8}) = f(\tfrac{7\pi}{8}) = 0.382683; \quad f(\tfrac{3\pi}{8}) = f(\tfrac{5\pi}{8}) = 0.923880.$$

$$\begin{aligned} T_1 &= T(f,\{0,\pi\}) = \pi\big(\tfrac{1}{2}f(0) + \tfrac{1}{2}f(\pi)\big) \\ &= \pi(\tfrac{1}{2}\cdot 0 + \tfrac{1}{2}\cdot 0) = \pi \cdot 0.000000 = 0.000000 \end{aligned}$$

$$\begin{aligned} T_2 &= T(f,\{0,\tfrac{\pi}{2},\pi\}) = \pi \cdot \tfrac{1}{2}\big(\tfrac{1}{2}f(0) + f(\tfrac{\pi}{2}) + \tfrac{1}{2}f(\pi)\big) \\ &= \pi \cdot \tfrac{1}{2}(\tfrac{1}{2}\cdot 0 + 1 + \tfrac{1}{2}\cdot 0) = \pi \cdot 0.500000 = 1.570796 \end{aligned}$$

$$\begin{aligned} T_4 &= T(f,\{0,\tfrac{\pi}{4},\tfrac{\pi}{2},\tfrac{3\pi}{4},\pi\}) = \pi \cdot \tfrac{1}{4}\big(\tfrac{1}{2}f(0) + f(\tfrac{\pi}{4}) + f(\tfrac{\pi}{2}) + f(\tfrac{3\pi}{4}) + \tfrac{1}{2}f(\pi)\big) \\ &= \pi \cdot \tfrac{1}{4}\big(\tfrac{1}{2}\cdot 0 + 0.707107 + 1 + 0.707107 + \tfrac{1}{2}\cdot 0\big) = \pi \cdot 0.603553 = 1.896119 \end{aligned}$$

$$\begin{aligned} T_8 &= T(f,\{0,\tfrac{\pi}{8},\tfrac{\pi}{4},\tfrac{3\pi}{8},\tfrac{\pi}{2},\tfrac{5\pi}{8},\tfrac{3\pi}{4},\tfrac{7\pi}{8},\pi\}) = \tfrac{1}{2}\big(T_4 + \tfrac{\pi}{4}\big(f(\tfrac{\pi}{8}) + f(\tfrac{3\pi}{8}) + f(\tfrac{5\pi}{8}) + f(\tfrac{7\pi}{8})\big)\big) \\ &= \tfrac{1}{2}\big(1.896119 + \pi \cdot \tfrac{1}{4}(0.382683 + 0.923880 + 0.923880 + 0.382683)\big) \\ &= \tfrac{1}{2}\big(1.896119 + \pi \cdot 0.653281\big) = \tfrac{1}{2}(1.896119 + 2.052344) = 1.974232 \end{aligned}$$

Romburg integration

Example Estimate $\int_0^\pi \sin x \, dx$ using Romburg integration computing $R_{3,3}$.

$$R_{0,0} = 0.000000; \quad R_{1,0} = 1.570796; \quad R_{2,0} = 1.896119; \quad R_{3,0} = 1.974232.$$

$$\begin{aligned} R_{1,1} &= R_{1,0} + \tfrac{1}{3}\big(R_{1,0} - R_{0,0}\big) = \tfrac{1}{3}\big(4R_{1,0} - R_{0,0}\big) \\ &= \tfrac{1}{3}(4 \times 1.570796 - 0.000000) = 2.094395 \\ R_{2,1} &= \tfrac{1}{3}\big(4R_{2,0} - R_{1,0}\big) = \tfrac{1}{3}(4 \times 1.896119 - 1.570796) = 2.004560 \\ R_{3,1} &= \tfrac{1}{3}\big(4R_{3,0} - R_{2,0}\big) = \tfrac{1}{3}(4 \times 1.974232 - 1.896119) = 2.000269 \end{aligned}$$

$$\begin{aligned} R_{2,2} &= R_{2,1} + \tfrac{1}{15}\big(R_{2,1} - R_{1,1}\big) = \tfrac{1}{15}\big(16R_{2,1} - R_{1,1}\big) \\ &= \tfrac{1}{15}(16 \times 2.004560 - 2.094395) = 1.998571 \\ R_{3,2} &= \tfrac{1}{15}\big(16R_{3,1} - R_{2,1}\big) = \tfrac{1}{15}(16 \times 2.000269 - 2.004560) = 1.999983 \end{aligned}$$

$$\begin{aligned} R_{3,3} &= R_{3,2} + \tfrac{1}{63}\big(R_{3,2} - R_{2,2}\big) = \tfrac{1}{64}\big(64R_{3,2} - R_{2,2}\big) \\ &= \tfrac{1}{63}(64 \times 1.999983 - 1.998571) = 2.000006 \end{aligned}$$

Romburg integration

Example Estimate $\int_0^\pi \sin x \, dx$ using Romburg integration computing $R_{3,3}$.

Computed Romburg estimates:

$R_{0,0} = T_1 = 0.000000$			
$R_{1,0} = T_2 = 1.570796$	$R_{1,1} = 2.094395$		
$R_{2,0} = T_4 = 1.896119$	$R_{2,1} = 2.004560$	$R_{2,2} = 1.998571$	
$R_{3,0} = T_8 = 1.974232$	$R_{3,1} = 2.000269$	$R_{3,2} = 1.999983$	$R_{3,3} = 2.000006$

So $\int_0^\pi \sin x \, dx \approx R_{4,4} = 2.000006$.

Exact answer 2.000000, relative error $3 \times 10^{-6} = 0.0003\%$!

Romburg integration

Exercise Estimate $\int_0^1 x^2\,dx$ by $R_{2,2}$.

Answer:

$$\begin{array}{lll} R_{0,0} = 0.50000 & & \\ R_{1,0} = 0.37500 & R_{1,1} = 0.333333 & \\ R_{2,0} = 0.34375 & R_{2,1} = 0.333333 & R_{2,2} = 0.333333 \end{array}$$

Exercise Estimate $\int_1^2 1/x\,dx = \ln 2 \approx 0.693147$ by $R_{2,2}$.

Answer:

$$\begin{aligned} &R_{0,0} = 3/4 = 0.750000 \\ &R_{2,0} = 17/24 = 0.708333 \\ &R_{2,0} = 1171/1680 = 0.697024 \\ &R_{1,1} = R_{1,0} + \tfrac{1}{3}(R_{1,0} - R_{0,0}) = 25/36 = 0.694444 \\ &R_{2,1} = R_{1,0} + \tfrac{1}{3}(R_{1,0} - R_{0,0}) = 1747/2520 = 0.693254 \\ &R_{2,2} = R_{2,1} + \tfrac{1}{15}(R_{2,1} - R_{1,1}) = 4367/6300 = 0.693175 \end{aligned}$$

Adaptive Integration

Adaptive integration

Adaptive Methods In practise, we wish to estimate $\int_a^b f(x)\,dx$ to some fixed tolerance ϵ.

Suppose we can find an estimate $E(f, [p, q])$ for an integration method over the interval $[p, q]$.

Then the total error for a partition $P = \{x_0, x_1, \ldots, x_n\}$ is approximately

$$\sum_{i=1}^{n} E(f, [x_{i-1}, x_i]).$$

We can *refine* the partition by splitting the subinterval with the largest error to obtain a (hopefully) better approximation.

Over a fixed subinterval $[p, q]$, the (average) error should be at most

$$\frac{q-p}{b-a}\,\epsilon$$

We can often estimate the error on subinterval $[p, q]$ using two evaluations of a simple integration scheme.

Adaptive trapezoid rule

Adaptive trapezoid rule Composite trapezoid rule; error $\frac{f''(\xi)(b-a)}{12}h^2$.

Assuming $f''(\xi)$ is approximately constant K, can estimate K using two evaluations of the trapezoid rule.

Recall $T_2(f,[a,b]) := T(f,[a,\frac{a+b}{2},b]) = T(f,[a,\frac{a+b}{2}]) + T(f,[\frac{a+b}{2},b])$, so

$$T(f,[a,b]) - I \approx \frac{f''(\xi)(b-a)}{12}h^2; \quad T_2(f,[a,b]) - I \approx \frac{f''(\tilde{\xi})(b-a)}{12}(h/2)^2.$$

Assuming $f''(\xi) \approx f''(\tilde{\xi}) \approx K$, we have

$$T_2(f,[a,b]) - I \approx \frac{K(b-a)}{12}(h/2)^2 \approx (T(f,[a,b]) - I)/4.$$

Multiplying through by 4, rearranging, and dividing by 3 gives

$$\tfrac{1}{3}\big(T_2(f,[a,b]) - T(f,[a,b])\big) \approx -(T_2(f,[a,b]) - I).$$

So we obtain error estimate on $[a,b]$ of

$$\begin{aligned}\epsilon = |T_2(f,[a,b]) - I| &\approx \tfrac{1}{3}|T(f,[a,\tfrac{a+b}{2},b]) - T(f,[a,b])| \\ &= \tfrac{1}{12}(b-a)\big|f(a) - 2f(\tfrac{a+b}{2}) + f(b)\big|.\end{aligned}$$

Adaptive trapezoid rule

Adaptive trapezoid rule Approximate the integral of f over $[p,q]$ by

$$\begin{aligned}\int_p^q f(x)\,dx &\approx T(f,[p,\tfrac{p+q}{2},q]) = T_2(f,[p,q]) \\ &= \frac{q-p}{4}\big(f(p) + 2f(\tfrac{p+q}{2}) + f(q)\big).\end{aligned}$$

Estimate the error of this approximation as

$$\begin{aligned}E_{T_2}(f,[p,q]) &\approx \tfrac{1}{3}\,|T(f,[p,\tfrac{p+q}{2},q]) - T(f,[p,q])| \\ &= \frac{q-p}{12}\big(f(p) - 2f(\tfrac{p+q}{2}) + f(q)\big)\end{aligned}$$

Subdivide the interval with the largest estimated error until the total estimated error is less than ϵ.

Alternatively, subdivide each interval $[p,q]$ if

$$E_{T_2}(f,[p,q]) > \frac{q-p}{b-a}\,\epsilon\,.$$

Adaptive trapezoid rule

Example Evaluate $\int_0^2 1/(3+x^4)\,dx$ with error $\epsilon = 10^{-2}$.

$T(f,[0,2]) \overset{4\,\text{dp}}{=} 0.3860,\ T(f,[0,1]){+}T(f,[1,2]) \overset{4\,\text{dp}}{=} 0.2917 + 0.1513 = 0.4430.$

$E_{T_2}(f,[0,2]) = 0.0190$ is too high, need to split.

$[p,q]$	$T(f,[p,q])$	$T_2(f,[p,q]) = T(f,[p,\frac{p+q}{2},q])$	$E_{T_2}(f,[p,q])$
$[0.0,2.0]$	0.3860	0.4430	0.0190
$[0.0,1.0]$	0.2917	0.3091	0.0058
$[1.0,2.0]$	0.1513	0.1377	0.0045
$[0.0,0.5]$	0.1650	0.1657	0.0002
$[0.5,1.0]$	0.1441	0.1474	0.0011

So use trapezoid rule with partition $P = [0.0, 0.25, 0.5, 0.75, 1.0, 1.5, 2.0]$.
Total estimated error $0.0011 + 0.0002 + 0.0045 = 0.0058\,(4\,\text{dp})$.
Estimate of integral

$$\begin{aligned}T(f,P) &= T(f,[0.0,0.25,0.5]) + T(f,[0.5,0.75,1.0]) + T(f,[1.0,1.5,2.0])\\ &\overset{4\,\text{dp}}{=} 0.1657 + 0.1474 + 0.1377 = 0.4508.\end{aligned}$$

Exact value $0.4486\,(4\,\text{dp})$; error $2.2\times10^{-3} < 10^{-2}$.

Adaptive Simpson's rule (Non-examinable)

Adaptive Simpson's rule Composite Simpson's rule; error $\frac{f^{(4)}(\xi)(b-a)}{180}h^4$. Assuming $f^{(4)}(\xi)$ is approximately constant K, can estimate K using two evaluations of Simpson's rule. Let $h = (b-a)/2$.

$$S(f,[a,b]) - I \approx \frac{f^{(4)}(\xi)(b-a)}{180}h^4;$$

$$S(f,[a,c]) + S(f,[c,b]) - I \approx \frac{f^{(4)}(\tilde{\xi})(b-a)}{180}(h/2)^4.$$

Assuming $f^{(4)}(\xi) \approx f^{(4)}(\tilde{\xi}) \approx K$, we have

$$S(f,[a,c]) + S(f,[c,b]) - I \approx \frac{K(b-a)}{180}(h/2)^4 \approx (S(f,[a,b]) - I)/16$$

Multiplying through by 16 and rearranging gives

$$S(f,[a,c]){+}S(f,[c,b]) - S(f,[a,b])) \approx -15(S(f,[a,c]){+}S(f,[c,b]) - I)$$

So we obtain error estimate on $[a,b]$ of

$$\begin{aligned}\epsilon = |S(f,[a,c]){+}S(f,[c,b]) - I| &\approx \tfrac{1}{15}|S(f,[a,c]){+}S(f,[c,b]) - S(f,[a,b])|\\ &= \tfrac{1}{180}(b-a)\big(f(a) - 4f(a+h) + 6f(a+2h) - 4f(a+3h) + f(a+4h)\big)\end{aligned}$$

Adaptive Simpson's rule (Non-examinable)

Adaptive Simpson's rule Approximate the integral of f over $[p,q]$ by

$$\int_p^q f(x)\,dx \approx S(f,[p,\tfrac{p+q}{2}]) + S(f,[\tfrac{p+q}{2},q])$$
$$= \frac{q-p}{12}\big(f(p)+4f(\tfrac{3p+q}{4})+2f(\tfrac{p+q}{2})+4f(\tfrac{p+3q}{4})+f(q)\big).$$

Estimate the error of this approximation as

$$E_S(f,[p,q]) \approx \tfrac{1}{15}\,|S(f,[p,\tfrac{p+q}{2}]) + S(f,[\tfrac{p+q}{2},q]) - S(f,p,q)|$$
$$= \frac{q-p}{180}\big(f(p)-4f(\tfrac{3p+q}{4})+6f(\tfrac{p+q}{2})-4f(\tfrac{p+3q}{4})+f(q)\big)$$

Subdivide the interval $[p,q]$ if

$$E_S(f,[p,q]) > \frac{q-p}{b-a}\,\epsilon\,.$$

Alternatively, subdivide the interval with the largest estimated error until the total estimated error is less than ϵ.

Adaptive Simpson's rule (Non-examinable)

Example Consider $\int_0^2 1/(1+x^2)\,dx$ with error $\epsilon = 10^{-4}$.
Estimate $S(f,[0,2]) = 1.066667$, $S(f,[0,1]) + S(f,[1,2]) = 1.105128$, $E_S(f,[0,2]) = 0.0025$. Too high, need to split.

$[p,q]$	$S(f,[p,q])$	$S(f,[p,r])+S(f,[r,q])$	$E_S(f,[p,q])$	$\frac{q-p}{b-a}\epsilon$
$[0.0,2.0]$	1.066667	1.105128	2.5×10^{-3}	1.0×10^{-4}
$[0.0,1.0]$	0.783333	0.785392	1.4×10^{-4}	5.0×10^{-5}
$[1.0,2.0]$	0.321795	0.321748	3.1×10^{-6}	5.0×10^{-5}
$[0.0,0.5]$	0.463725	0.46365	4.8×10^{-6}	2.5×10^{-5}
$[0.5,1.0]$	0.321667	0.321745	5.3×10^{-6}	2.5×10^{-5}

So use Simpson's rule with partition

$$P = [0.0, 0.25, 0.5, 0.75, 1.0, 1.5, 2.0],$$

evaluation points

$$[0.0, 0.125, 0.25, 0.375, 0.5, 0.625, 0.75, 0.875, 1.0, 1.25, 1.5, 1.75, 2.0]$$

Estimate of integral 1.107146; exact value 1.107149; error 2.6×10^{-6}.