Simpson's rule

Let f be approximated by a poly $p_2(x)$ of degree ≤ 2 passing through $(a, f(a)), (m, f(m)), (b, f(b))$, where $m = \frac{a+b}{2}$.
Let $p_2(x) = \frac{(x-m)(x-b)}{(a-m)(a-b)} f(a) + \frac{(x-a)(x-b)}{(m-a)(m-b)} f(m)$ $+ \frac{(x-a)(x-m)}{(b-a)(b-m)} f(b)$. Then

$$\begin{aligned}
I &= \int_a^b f(x)dx \\
&\approx \int_a^b p_2(x)dx \\
&= f(a)\frac{\int_a^b (x-m)(x-b)dx}{(a-m)(a-b)} + f(m)\frac{\int_a^b (x-a)(x-b)dx}{(m-a)(m-b)} \\
&\quad + f(b)\frac{\int_a^b (x-a)(x-m)dx}{(b-a)(b-a)} \\
&= f(a)\frac{(b-a)^3/12}{(b-a)^2/2} + f(m)\frac{(b-a)^3/6}{(b-a)^2/4} + f(b)\frac{(b-a)^3/12}{(b-a)^2/2} \\
&= \frac{b-a}{6}[f(a) + 4f(m) + f(b)]
\end{aligned}$$

We denote Simpson's rule by $S_a^b(f)$. By construction, Simpson's rule has poly degree at least 2.

Consider $f(x) = x^3$.
$I = \int_a^b x^3 dx = \frac{x^4}{4}|_a^b = \frac{b^4 - a^4}{4}$.
$Q = S_a^b(x^3) = \frac{b-a}{6}[a^3 + 4(\frac{a+b}{2})^3 + b^3] = \frac{b^4-a^4}{4}$.
Thus, Simpson's rule is exact for $f(x) = x^3$ for arbitrary a, b. To show that Simpson's is exact on any poly of degree 3 we first note that Simpson's rule is *linear*.

$$S_a^b(\alpha f + \beta g) = \alpha S_a^b(f) + \beta S_a^b(g)$$

for any functions f, g and scalars α, β and any interval $[a, b]$.

Let $p(x) = a_3x^3 + a_2x^2 + a_1x + a_0 = a_3x^3 + q(x)$, where $q(x)$ has degree ≤ 2.

$$\begin{aligned}
I &= \int_a^b p(x)dx \\
&= a_3 \int_a^b x^3 dx + \int_a^b q(x)dx \\
&= a_3 S_a^b(x^3) + S_a^b(q(x)) \\
&= S_a^b(a_3x^3 + q(x)) = S_a^b(p(x))
\end{aligned}$$

Thus, Simpson's is exact on $p(x)$. Finally, consider $f(x) = x^4$ and $a = 0, b = 1$.
$I = \int_0^1 x^4 dx = \frac{x^5}{5}|_0^1 = \frac{1}{5}$.
$S_0^1(x^4) = \frac{1}{6}[0 + 4(\frac{1}{2})^4 + 1] = \frac{5}{24} \neq \frac{1}{5}$. Thus, Simpson's is not exact for x^4 on $[0, 1]$. Therefore, it has poly degree 3.

Error in Simpson's rule

If we try to integrate $f(x) - p_2(x) = \frac{f^{(3)}(\xi)}{3!}(x - a)(x - m)(x - b)$, we note that $(x - a)(x - m)(x - b)$ does not have constant sign in $[a, b]$. Therefore, we cannot apply the MVT.

To get around this, consider the poly interpolant $p_3(x)$ of degree ≤ 3 that matches the data $(a, f(a)), (m, f(m)), (b, f(b))$ and its derivative matches $(m, f'(m))$. We can show that $p_3(x)$ exists and that
$f(x) - p_3(x) = \frac{f^{(4)}(\xi)}{4!}(x - a)(x - m)^2(x - b)$.
We have

$$\begin{aligned}
&\int_a^b f(x)dx - \int_a^b p_3(x)dx = \\
&\frac{1}{4!}\int_a^b f^{(4)}(\xi)(x - a)(x - m)^2(x - b)dx
\end{aligned}$$

Since $(x-a)(x-m)^2(x-b) \le 0$ in $[a,b]$, we can apply MVT.

$\int_a^b f(x)dx - \int_a^b p_3(x)dx$
$= \frac{f^{(4)}(\eta)}{4!}\int_a^b (x-a)(x-m)^2(x-b)dx$
$= -f^{(4)}(\eta)\frac{(b-a)^5}{2880}$

Since Simpson's has poly degree 3,
$\int_a^b p_3(x)dx = S_a^b(p_3(x))$ and hence,

$$\begin{aligned} S_a^b(p_3) &= \frac{b-a}{6}(p_3(a)+4p_3(m)+p_3(b)) \\ &= \frac{b-a}{6}(f(a)+4f(m)+f(b)) \\ &= S_a^b(f) \end{aligned}$$

Thus,

$\int_a^b f(x)dx - \frac{b-a}{6}(f(a)+4f(m)+f(b))$
$= -f^{(4)}(\eta)\frac{(b-a)^5}{2880}$

Corrected trapezoidal rule

Let f be approximated by a poly $p_3(x)$ of degree ≤ 3 which matches the data $(a,f(a)),(b,f(b))$ and the derivative data $(a,f'(a)),(b,f'(b))$, ie. $p_3(x)$ is the Hermite poly interpolant of degree ≤ 3. Then

$$I = \int_a^b f(x)dx \approx \int_a^b p_3(x)dx$$

Note that $\int_a^b p_3(x)dx = S_a^b(p_3)$(since Simpson's is exact on p_3)

$= \frac{b-a}{6}[p_3(a)+4p_3(\frac{a+b}{2})+p_3(b)]$
$= \frac{b-a}{6}[f(a)+$
$4[\frac{1}{2}(f(a)+f(b))+\frac{b-a}{8}(f'(a)-f'(b))]+f(b)]$
$= \frac{b-a}{2}(f(a)+f(b))+\frac{(b-a)^2}{12}(f'(a)-f'(b))$

Corrected trapezoidal rule $= CT_a^b(f)$. The CT rule has poly degree exactly 3.

Error in the CT rule

From the Hermite poly interp error formula

$$f(x)-p_3(x) = \frac{f^{(4)}(\xi)}{4!}(x-a)^2(x-b)^2$$

Hence,

$\int_a^b f(x)dx - \int_a^b p_3(x)dx$
$= \frac{1}{4!}\int_a^b f^{(4)}(\xi)(x-a)^2(x-b)^2dx$

Note that $(x-a)^2(x-b)^2$ does not change sign and assume that $f^{(4)}$ is cts. Apply MVT

$\int_a^b f(x)dx - \int_a^b p_3(x)dx$
$= \frac{1}{4!}f^{(4)}(\eta)\int_a^b (x-a)^2(x-b)^2dx$
$= f^{(4)}(\eta)\frac{(b-a)^5}{4!30}$
$= f^{(4)}(\eta)\frac{(b-a)^5}{720}$

Newton-Cotes quadrature rules

Quadrature rules with equally spaced nodes x_i are called **Newton-Cotes**, NC, rules.
Rules that include a and b as nodes are called **closed** NC rules, i.e. $x_i = a+ih$, $i=0,\ldots,n$ $h=\frac{b-a}{n}$.
Rules that do not include a or b as nodes are called **open** NC rules, i.e. $x_i = a+(i+1)h$, $i=0,\ldots,n$ $h=\frac{b-a}{n+2}$.

Though picking equidistant nodes seems natural and simple, it is not necessarily the best choice. The weights of a NC rule are often of varying sign and grow without bound as n increases. For these reasons, NC rules with large n are not used in practice.

If n is even (i.e. odd no. of data) and $f \in \mathbf{C}^{n+2}[a,b]$, the closed NC rule is degree $n+1$ and the error is

$$I - Q = \frac{h^{n+3} f^{(n+2)}(\eta)}{(n+2)!} C_n, \quad C_n = \int_0^n t^2(t-1)\cdots(t-n)dt$$

If n is odd (i.e. even no. of data) and $f \in \mathbf{C}^{n+1}[a,b]$, the closed NC rule is degree n and the error is

$$I - Q = \frac{h^{n+2} f^{(n+1)}(\eta)}{(n+1)!} \hat{C}_n, \quad \hat{C}_n = \int_0^n t(t-1)\cdots(t-n)dt$$

Compound quadrature rules

In order to increase the accuracy of integral approximations, we would need to increase the number of data pts. Since NC rules with more than 10 pts suffer from divergence (unbounded weights) and computational instability (varying sign), we try alternatives.

One alternative is to divide up the interval of integration into subintervals, called **panels**, and apply the same low degree rule over each subinterval.

Since the error of all NC rules is proportional to a power of the length of the interval $b-a$, we expect that it gets smaller as the length of the interval gets smaller.

A **compound** (**composite, repeated**) quadrature rule uses the same (simple and usually low n) rule for each panel.

Composite midpoint rule

Let s be the number of panels and $h = \frac{b-a}{s}$ the stepsize. Let $t_i = a + ih$, $i = 0, \ldots, s$ ($t_0 = a, t_s = b$).

$$\begin{aligned} I &= \int_a^b f(x)dx = \sum_{i=1}^{s} \int_{t_{i-1}}^{t_i} f(x)dx \\ &\approx \sum_{i=1}^{s} f\left(\frac{t_{i-1}+t_i}{2}\right)(t_i - t_{i-1}) \\ &= h \sum_{i=1}^{s} f(a + (i-1/2)h) \end{aligned}$$

This is equivalent to approximating f by a piecewise constant poly defined wrt to the knots t_i and integrating it. Note, this rule uses s function evaluations.

Error in the composite midpt rule

Total error:

$$\begin{aligned} &\int_a^b f(x)dx - h\sum_{i=1}^{s} f(a + (i-1/2)h) \\ = &\sum_{i=1}^{s} f''(\eta_i)\frac{h^3}{24} = \frac{h^3}{24}\sum_{i=1}^{s} f''(\eta_i), \end{aligned}$$

where η_i is an unknown pt in $[t_{i-1}, t_i]$.

MVT for sums

Let $f(x)$ be cts on $[a,b]$, let $x_1, \ldots, x_n \in [a,b]$ and let $w_1, \ldots, w_n$ be all of the same sign. Then

$$\sum_{i=1}^{n} w_i f(x_i) = f(\eta) \sum_{i=1}^{n} w_i, \eta \in [a,b]$$

Thus,

$$\begin{aligned} \frac{h^3}{24}\sum_{i=1}^{s} 1 \cdot f''(\eta_i) &= \frac{h^3}{24} s f''(\eta) \\ &= \frac{h^2}{24}\frac{b-a}{s} s f''(\eta) \\ &= \frac{(b-a)h^2}{24} f''(\eta) \end{aligned}$$

Compare the midpt rule error with composite midpt rule error

$$\frac{(b-a)^3}{24} f''(\eta) \qquad \frac{(b-a)h^2}{24} f''(\eta)$$

• The composite error is proportional to the length of the interval $b-a$.
• The error is 0 if $f(x)$ is a poly of degree ≤ 1.
• The error is 0 if $f(x)$ is a piecewise poly of degree ≤ 1 defined wrt the knots t_i.
• The error converges to 0 as $s \to \infty$.
• If we double the number of panels, we expect the error to decrease roughly by a factor of 4. (if we assume f'' does not vary a lot)

Other composite quadrature rules

Composite trapezoidal
It uses piecewise linear interpolation with function evaluation at each t_i, $i = 0, \ldots, s$. $f(t_i)$, $i = 1, \ldots, s-1$, is shared by 2 panels.

Composite Simpson
It uses piecewise quadratic interpolation with function evaluation at each t_i , $i = 0, \ldots, s$ and each midpt $\frac{t_{i-1}+t_i}{2}$, $i = 1, \ldots, s$ for a total of $2s+1$ function evaluations. $f(t_i)$, $i = 1, \ldots, s-1$, is shared by 2 panels.

Composite corrected trapezoidal
It uses piecewise Hermite cubic interpolation. The number of function evaluations is the same as composite trapezoidal with the addition of $\frac{h^2}{12}(f'(a) - f'(b))$–the rest of the derivative terms cancel out.

