SIMPSON'S RULE ERROR FORMULA

Recall the general Simpson's rule

$$\int_a^b f(x)\,dx \approx S_n(f) \equiv \frac{h}{3}\,[f(x_0) + 4f(x_1) + 2f(x_2)$$
$$+4f(x_3) + 2f(x_4) + \cdots$$
$$+2f(x_{n-2}) + 4f(x_{n-1}) + f(x_n)]$$

For its error, we have

$$E_n^S(f) \equiv \int_a^b f(x)\,dx - S_n(f) = -\frac{h^4\,(b-a)}{180} f^{(4)}(c_n)$$

for some $a \le c_n \le b$, with c_n otherwise unknown. For an asymptotic error estimate,

$$\int_a^b f(x)\,dx - S_n(f) \approx \widetilde{E}_n^S(f) \equiv -\frac{h^4}{180}\left[f'''(b) - f'''(a)\right]$$

DISCUSSION

For Simpson's error formula, both formulas assume that the integrand $f(x)$ has four continuous derivatives on the interval $[a, b]$. What happens when this is not valid?

Both formulas also say the error should decrease by a factor of around 16 when n is doubled.

Compare these results with those for the trapezoidal rule error formulas:.

$$E_n^T(f) \equiv \int_a^b f(x)\,dx - T_n(f) = -\frac{h^2\,(b-a)}{12} f''\,(c_n)$$

$$E_n^T(f) \approx -\frac{h^2}{12}\Big[f'(b) - f'(a)\Big] \equiv \widetilde{E}_n^T(f)$$

EXAMPLE

Consider evaluating

$$I = \int_0^2 \frac{dx}{1 + x^2}$$

using Simpson's rule $S_n(f)$. How large should n be chosen in order to ensure that

$$\left| E_n^S(f) \right| \leq 5 \times 10^{-6}$$

Begin by noting that

$$\begin{aligned} f^{(4)}(x) &= 24 \frac{5x^4 - 10x^2 + 1}{\left(1 + x^2\right)^5} \\ \max_{0 \leq x \leq 1} \left| f^{(4)}(x) \right| &= f^{(4)}(0) = 24 \end{aligned}$$

Then

$$\begin{aligned} E_n^S(f) &= -\frac{h^4 (b - a)}{180} f^{(4)}(c_n) \\ \left| E_n^S(f) \right| &\leq \frac{h^4 \cdot 2}{180} \cdot 24 = \frac{4h^4}{15} \end{aligned}$$

Then $\left|E_n^S(f)\right| \leq 5 \times 10^{-6}$ is true if

$$\begin{aligned}\frac{4h^4}{15} &\leq 5 \times 10^{-6} \\ h &\leq .0658 \\ n &\geq 30.39\end{aligned}$$

Therefore, choosing $n \geq 32$ will give the desired error bound. Compare this with the earlier trapezoidal example in which $n \geq 517$ was needed.

For the asymptotic error estimate, we have

$$f'''(x) = -24x\frac{x^2 - 1}{\left(1 + x^2\right)^4}$$

$$\begin{aligned}\widetilde{E}_n^S(f) &\equiv -\frac{h^4}{180}\left[f'''(2) - f'''(0)\right] \\ &= \frac{h^4}{180} \cdot \frac{144}{625} = \frac{4}{3125}h^4\end{aligned}$$

INTEGRATING sqrt(x)

Consider the numerical approximation of

$$\int_0^1 \text{sqrt}(x)\, dx = \frac{2}{3}$$

In the following table, we give the errors when using both the trapezoidal and Simpson rules.

n	E_n^T	$Ratio$	E_n^S	$Ratio$
2	$6.311E-2$		$2.860E-2$	
4	$2.338E-2$	2.70	$1.012E-2$	2.82
8	$8.536E-3$	2.74	$3.587E-3$	2.83
16	$3.085E-3$	2.77	$1.268E-3$	2.83
32	$1.108E-3$	2.78	$4.485E-4$	2.83
64	$3.959E-4$	2.80	$1.586E-4$	2.83
128	$1.410E-4$	2.81	$5.606E-5$	2.83

The rate of convergence is slower because the function $f(x) =$sqrt(x) is not sufficiently differentiable on $[0,1]$. Both methods converge with a rate proportional to $h^{1.5}$.

ASYMPTOTIC ERROR FORMULAS

If we have a numerical integration formula,

$$\int_a^b f(x)\,dx \approx \sum_{j=0}^{n} w_j f(x_j)$$

let $E_n(f)$ denote its error,

$$E_n(f) = \int_a^b f(x)\,dx - \sum_{j=0}^{n} w_j f(x_j)$$

We say another formula $\widetilde{E}_n(f)$ is an asymptotic error formula this numerical integration if it satisfies

$$\lim_{n\to\infty} \frac{\widetilde{E}_n(f)}{E_n(f)} = 1$$

Equivalently,

$$\lim_{n\to\infty} \frac{E_n(f) - \widetilde{E}_n(f)}{E_n(f)} = 0$$

These conditions say that $\widetilde{E}_n(f)$ looks increasingly like $E_n(f)$ as n increases, and thus

$$E_n(f) \approx \widetilde{E}_n(f)$$

EXAMPLE. For the trapezoidal rule,

$$E_n^T(f) \approx \widetilde{E}_n^T(f) \equiv -\frac{h^2}{12}\left[f'(b) - f'(a)\right]$$

This assumes $f(x)$ has two continuous derivatives on the interval $[a, b]$.

EXAMPLE. For Simpson's rule,

$$E_n^S(f) \approx \widetilde{E}_n^S(f) \equiv -\frac{h^4}{180}\left[f'''(b) - f'''(a)\right]$$

This assumes $f(x)$ has four continuous derivatives on the interval $[a, b]$.

Note that both of these formulas can be written in an equivalent form as

$$\widetilde{E}_n(f) = \frac{c}{n^p}$$

for appropriate constant c and exponent p. With the trapezoidal rule, $p = 2$ and

$$c = -\frac{(b-a)^2}{12}\left[f'(b) - f'(a)\right]$$

and for Simpson's rule, $p = 4$ with a suitable c.

The formula

$$\widetilde{E}_n(f) = \frac{c}{n^p} \qquad (*)$$

occurs for other many numerical integration formulas that we have not yet defined or studied. In addition, if we use the trapezoidal or Simpson rules with an integrand $f(x)$ which is not sufficiently differentiable, then $(*)$ may hold with an exponent p that is less than the ideal.

<u>EXAMPLE</u>. Consider

$$I = \int_0^1 x^\beta \, dx$$

in which $-1 < \beta < 1$, $\beta \neq 0$. Then the convergence of the trapezoidal rule can be shown to have an asymptotic error formula

$$E_n \approx \widetilde{E}_n = \frac{c}{n^{\beta+1}} \qquad (**)$$

for some constant c dependent on β. A similar result holds for Simpson's rule, with $-1 < \beta < 3$, β not an integer. We can actually specify a formula for c; but the formula is often less important than knowing that $(**)$ is valid for some c.

APPLICATION OF ASYMPTOTIC ERROR FORMULAS

Assume we know that an asymptotic error formula

$$I - I_n \approx \frac{c}{n^p}$$

is valid for some numerical integration rule denoted by I_n. Initially, assume we know the exponent p. Then imagine calculating both I_n and I_{2n}. With I_{2n}, we have

$$I - I_{2n} \approx \frac{c}{2^p n^p}$$

This leads to

$$\begin{aligned} I - I_n &\approx 2^p \left[I - I_{2n} \right] \\ I &\approx \frac{2^p I_{2n} - I_n}{2^p - 1} = I_{2n} + \frac{I_{2n} - I_n}{2^p - 1} \end{aligned}$$

The formula

$$I \approx I_{2n} + \frac{I_{2n} - I_n}{2^p - 1} \qquad (**)$$

is called Richardson's extrapolation formula.

EXAMPLE. With the trapezoidal rule and with the integrand $f(x)$ having two continuous derivatives,

$$I \approx T_{2n} + \frac{1}{3}[T_{2n} - T_n]$$

EXAMPLE. With Simpson's rule and with the integrand $f(x)$ having four continuous derivatives,

$$I \approx S_{2n} + \frac{1}{15}[S_{2n} - S_n]$$

We can also use the formula $(**)$ to obtain error estimation formulas:

$$I - I_{2n} \approx \frac{I_{2n} - I_n}{2^p - 1} \qquad (**)$$

This is called Richardson's error estimate. For example, with the trapezoidal rule,

$$I - T_{2n} \approx \frac{1}{3}[T_{2n} - T_n]$$

These formulas are illustrated for the trapezoidal rule in an accompanying table, for

$$\int_0^{\pi} e^x \cos x \, dx = -\frac{e^{\pi} + 1}{2} \doteq -12.07034632$$

AITKEN EXTRAPOLATION

In this case, we again assume

$$I - I_n \approx \frac{c}{n^p}$$

But in contrast to previously, we do not know either c or p. Imagine computing I_n, I_{2n}, and I_{4n}. Then

$$\begin{aligned} I - I_n &\approx \frac{c}{n^p} \\ I - I_{2n} &\approx \frac{c}{2^p n^p} \\ I - I_{4n} &\approx \frac{c}{4^p n^p} \end{aligned}$$

We can directly try to estimate I. Dividing

$$\frac{I - I_n}{I - I_{2n}} \approx 2^p \approx \frac{I - I_{2n}}{I - I_{4n}}$$

Solving for I, we obtain

$$\begin{aligned} (I - I_{2n})^2 &\approx (I - I_n)(I - I_{4n}) \\ I(I_n + I_{4n} - 2I_{2n}) &\approx I_n I_{4n} - I_{2n}^2 \\ I &\approx \frac{I_n I_{4n} - I_{2n}^2}{I_n + I_{4n} - 2I_{2n}} \end{aligned}$$

This can be improved computationally, to avoid loss of significance errors.

$$\begin{aligned} I &\approx I_{4n} + \left[\frac{I_n I_{4n} - I_{2n}^2}{I_n + I_{4n} - 2I_{2n}} - I_{4n} \right] \\ &= I_{4n} - \frac{(I_{4n} - I_{2n})^2}{(I_{4n} - I_{2n}) - (I_{2n} - I_n)} \end{aligned}$$

This is called <u>Aitken's extrapolation formula</u>.

To estimate p, we use

$$\frac{I_{2n} - I_n}{I_{4n} - I_{2n}} \approx 2^p$$

To see this, write

$$\frac{I_{2n} - I_n}{I_{4n} - I_{2n}} = \frac{(I - I_n) - (I - I_{2n})}{(I - I_{2n}) - (I - I_{4n})}$$

Then substitute from the following and simplify:

$$\begin{aligned} I - I_n &\approx \frac{c}{n^p} \\ I - I_{2n} &\approx \frac{c}{2^p n^p} \\ I - I_{4n} &\approx \frac{c}{4^p n^p} \end{aligned}$$

EXAMPLE. Consider the following table of numerical integrals. What is its order of convergence?

n	I_n	$I_n - I_{\frac{1}{2}n}$	$Ratio$
2	.28451779686		
4	.28559254576	$1.075E-3$	
8	.28570248748	$1.099E-4$	9.78
16	.28571317731	$1.069E-5$	10.28
32	.28571418363	$1.006E-6$	10.62
64	.28571427643	$9.280E-8$	10.84

It appears

$$2^p \doteq 10.84, \qquad p \doteq \log_2 10.84 = 3.44$$

We could now combine this with Richardson's error formula to estimate the error:

$$I - I_n \approx \frac{1}{2^p - 1}\left[I_n - I_{\frac{1}{2}n}\right]$$

For example,

$$I - I_{64} \approx \frac{1}{2.44}\left[9.280E-8\right] = 3.803E-8$$

PERIODIC FUNCTIONS

A function $f(x)$ is <u>periodic</u> if the following condition is satisfied. There is a smallest real number $\tau > 0$ for which

$$f(x+\tau) = f(x), \qquad -\infty < x < \infty, \quad (*)$$

The number τ is called the <u>period</u> of the function $f(x)$. The constant function $f(x) \equiv 1$ is also considered periodic, but it satisfies this condition with any $\tau > 0$. Basically, a periodic function is one which repeats itself over intervals of length τ.

The condition $(*)$ implies

$$f^{(m)}(x+\tau) = f^{(m)}(x), \qquad -\infty < x < \infty, \quad (*)$$

for the m^{th}-derivative of $f(x)$, provided there is such a derivative. Thus the derivatives are also periodic.

Periodic functions occur very frequently in applications of mathematics, reflecting the periodicity of many phenomena in the physical world.

PERIODIC INTEGRANDS

Consider the special class of integrals

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

in which $f(x)$ is periodic, with $b-a$ an integer multiple of the period τ for $f(x)$. In this case, the performance of the trapezoidal rule and other numerical integration rules is much better than that predicted by earlier error formulas.

To hint at this improved performance, recall

$$\int_a^b f(x)\, dx - T_n(f) \approx \widetilde{E}_n(f) \equiv -\frac{h^2}{12}\left[f'(b) - f'(a)\right]$$

With our assumption on the periodicity of $f(x)$, we have

$$f(a) = f(b), \qquad f'(a) = f'(b)$$

Therefore,

$$\widetilde{E}_n(f) = 0$$

and we should expect improved performance in the convergence behaviour of the trapezoidal sums $T_n(f)$.

If in addition to being periodic on $[a, b]$, the integrand $f(x)$ also has m continous derivatives, then it can be shown that

$$I(f) - T_n(f) = \frac{c}{n^m} + \text{ smaller terms}$$

By "smaller terms", we mean terms which decrease to zero more rapidly than n^{-m}.

Thus if $f(x)$ is periodic with $b - a$ an integer multiple of the period τ for $f(x)$, and if $f(x)$ is infinitely differentiable, then the error $I - T_n$ decreases to zero more rapidly than n^{-m} for any $m > 0$. For periodic integrands, the trapezoidal rule is an optimal numerical integration method.

EXAMPLE. Consider evaluating

$$I = \int_0^{2\pi} \frac{\sin x \, dx}{1 + e^{\sin x}}$$

Using the trapezoidal rule, we have the results in the following table. In this case, the formulas based on Richardson extrapolation are no longer valid.

n	T_n	$T_n - T_{\frac{1}{2}n}$
2	0.0	
4	−0.72589193317292	$-7.259E-1$
8	−0.74006131211583	$-1.417E-2$
16	−0.74006942337672	$-8.111E-6$
32	−0.74006942337946	$-2.746E-12$
64	−0.74006942337946	0.0