

An Euler-Maclaurin-like summation formula for Simpson's rule

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One of the most popular numerical integration formulas is the composite Simpson's rule, which is derived in every numerical analysis textbook (and many Calculus texts) as

$$\int_a^b f(x) dx = \frac{h}{3} \left[f(x_0) + 2 \sum_{j=1}^{n/2-1} f(x_{2j}) + 4 \sum_{j=1}^{n/2} f(x_{2j-1}) + f(x_n) \right] - \frac{(b-a)h^4}{180} f^{(4)}(\xi), \quad (1)$$

where n is even, $h = (b-a)/n$, $x_i = a + ih$, and $\xi \in (a, b)$. We usually derive (1) using Lagrange polynomials or making the formula exact for $f(x) = 1, x, x^2$. A standard exercise for a numerical analysis class is to use the composite Simpson's rule to approximate an integral with n equal to successive powers of two, and verify that (as long as the fourth derivative of f is well behaved) the errors reduce by a factor of sixteen due to the h^4 term.

Recently I assigned this exercise with the integral $\int_0^1 \frac{4 dx}{1+x^2} = \pi$. Imagine my surprise when the ratio of errors was not sixteen as expected, but sixty four! Clearly in this case the h^4 error term has been eliminated and the error is in fact order h^6 . But why?

What follows resurrects an alternative form of the error term for Simpson's rule, and uses it to explain the behavior of this integral. In the process a new derivation of the Euler-Maclaurin summation formulas follow naturally. The derivation is then extended to derive an Euler-Maclaurin-like formula for

Simpson's rule. The first Euler-Maclaurin summation formula (for example equation 21.1.30 of Abramowitz and Stegun [1]) can be written as

$$\begin{aligned} \int_a^b f(x) dx &= \frac{h}{2} \left[f(a) + 2 \sum_{k=1}^{n-1} f(a + kh) + f(b) \right] \\ &\quad - \sum_{k=1}^{m-1} \frac{h^{2k} B_{2k}}{(2k)!} [f^{(2k-1)}(b) - f^{(2k-1)}(a)] \\ &\quad - \frac{h^{2m+1} B_{2m}}{(2m)!} \sum_{k=0}^{n-1} f^{(2m)}(a + kh + \theta h), \end{aligned} \quad (2)$$

where the first $2m$ derivatives of f are continuous on (a, b) , $h = (b - a)/n$, and $\theta \in (0, 1)$. In the case that f is analytic and its derivatives do not grow too quickly, the error term can be removed and the second last summation extended to infinity.

Standard rules, nonstandard error terms

Consider approximating $\int_{x_0}^{x_2} f(x) dx$, where $x_i = x_0 + ih$ and $h = x_i - x_{i-1}$. In this case the number of intervals, n , equals two. For simplicity we shall assume that f is analytic. Let us start with Taylor's series for $f(x)$ around x_1 ,

$$f(x) = f(x_1) + \sum_{k=1}^{\infty} \frac{(x - x_1)^k}{k!} f^{(k)}(x_1).$$

Integrating from x_0 to x_2 gives

$$\begin{aligned} \int_{x_0}^{x_2} f(x) dx &= f(x_1) \int_{x_0}^{x_2} dx + \sum_{k=1}^{\infty} \frac{f^{(k)}(x_1)}{k!} \int_{x_0}^{x_2} (x - x_1)^k dx \\ &= (x_2 - x_0) f(x_1) + \sum_{k=1}^{\infty} \frac{f^{(k)}(x_1)}{k!} \left[\frac{(x - x_1)^{k+1}}{k+1} \right]_{x_0}^{x_2} \\ &= 2h f(x_1) + \sum_{k=1}^{\infty} \frac{f^{(k)}(x_1)}{(k+1)!} (h^{k+1} - (-h)^{k+1}), \end{aligned}$$

and since the even terms in the summation cancel, we have

$$\int_{x_0}^{x_2} f(x) dx = 2hf(x_1) + \sum_{k=1}^{\infty} \frac{2h^{2k+1}}{(2k+1)!} f^{(2k)}(x_1). \quad (3)$$

This is just the midpoint rule, but with a nonstandard error term. Usually the error term is written as $h^3 f''(\xi)/3$ where $\xi \in (x_0, x_2)$.

Let us now evaluate the Taylor series at x_0 and x_2 , giving

$$f(x_0) = f(x_1) + \sum_{k=1}^{\infty} \frac{(-1)^k h^k}{k!} f^{(k)}(x_1), \quad \text{and} \quad (4)$$

$$f(x_2) = f(x_1) + \sum_{k=1}^{\infty} \frac{h^k}{k!} f^{(k)}(x_1). \quad (5)$$

Adding (4) and (5) cancels the terms in the sum with odd powers of h , and multiplying the sum by h gives

$$h[f(x_0) + f(x_2)] = 2hf(x_1) + \sum_{k=1}^{\infty} \frac{2h^{2k+1}}{(2k)!} f^{(2k)}(x_1). \quad (6)$$

Substituting $2hf(x_1)$ from (3) gives

$$\begin{aligned} \int_{x_0}^{x_2} f(x) dx &= h[f(x_0) + f(x_2)] - \sum_{k=1}^{\infty} \frac{2h^{2k+1}}{(2k)!} f^{(2k)}(x_1) \\ &\quad + \sum_{k=1}^{\infty} \frac{2h^{2k+1}}{(2k+1)!} f^{(2k)}(x_1) \\ &= h[f(x_0) + f(x_2)] - \sum_{k=1}^{\infty} \frac{4kh^{2k+1}}{(2k+1)!} f^{(2k)}(x_1), \end{aligned} \quad (7)$$

using $1/(2k+1)! - 1/(2k)! = -2k/(2k+1)!$. This is the trapezoidal rule on the interval $[x_0, x_2]$, again with a nontraditional error term. The trapezoidal rule is usually given on $[x_0, x_1]$ with error term $-h^3 f''(\xi)/12$. Transforming to the interval $[x_0, x_2]$ of width $2h$ changes the error term to $-2h^3 f''(\xi)/3$. Note that this method of deriving the midpoint and trapezoidal rules can be found in Heath [2], but with less detail in stating the error terms.

Now if we add $4hf(x_1)$ to both sides of (6) and divide by 3, then substitute for $2hf(x_1)$ on the right hand side, we have

$$\begin{aligned} \frac{h}{3}[f(x_0) + 4f(x_1) + f(x_2)] &= \int_{x_0}^{x_2} f(x) dx - \sum_{k=1}^{\infty} \frac{2h^{2k+1}}{(2k+1)!} f^{(2k)}(x_1) \\ &\quad + \sum_{k=1}^{\infty} \frac{2h^{2k+1}}{3(2k)!} f^{(2k)}(x_1), \end{aligned}$$

or

$$\begin{aligned} \int_{x_0}^{x_2} f(x) dx &= \frac{h}{3}[f(x_0) + 4f(x_1) + f(x_2)] \\ &\quad + \sum_{k=1}^{\infty} 2h^{2k+1} \left(\frac{1}{(2k+1)!} - \frac{1}{3(2k)!} \right) f^{(2k)}(x_1), \end{aligned}$$

so

$$\int_{x_0}^{x_2} f(x) dx = \frac{h}{3}[f(x_0) + 4f(x_1) + f(x_2)] - \sum_{k=2}^{\infty} \frac{4(k-1)h^{2k+1}}{3(2k+1)!} f^{(2k)}(x_1), \quad (8)$$

where the sum starts at $k = 2$ since the $k = 1$ term is zero. This is Simpson's rule with a nontraditional error term, which I have not seen in either numerical integration or general numerical analysis texts. In fact, it was stated in 1926 by Scarborough [3], but does not appear to have been taken up by the numerical analysis community.

In principle, there is no reason why this method could not be used to derive the complete family of Newton-Cotes integration formulas. Taylor series around other x_i can be combined with arbitrary multiplicative constants and the midpoint rule (3), and the constants can be chosen so that as many terms in the error expansion as possible are eliminated.

Composite rules If we let $h = (b - a)/n$, $x = a + ih$, and require n to be even, then $\int_a^b f(x) dx = \int_{x_0}^{x_n} f(x) dx = \sum_{j=1}^{n/2} \int_{x_{2j-2}}^{x_{2j}} f(x) dx$. Using (3), (7) and (8) for the individual integrals lead to the composite midpoint, trapezoidal

and Simpson's rules with nontraditional error terms as

$$\int_a^b f(x) dx = 2h \sum_{j=1}^{n/2} f(x_{2j-1}) + \sum_{k=1}^{\infty} \frac{2h^{2k+1}}{(2k+1)!} \sum_{j=1}^{n/2} f^{(2k)}(x_{2j-1}), \quad (9)$$

$$\int_a^b f(x) dx = h \left[f(x_0) + 2 \sum_{j=1}^{n/2-1} f(x_{2j}) + f(x_n) \right] - \sum_{k=1}^{\infty} \frac{4kh^{2k+1}}{(2k+1)!} \sum_{j=1}^{n/2} f^{(2k)}(x_{2j-1}), \quad \text{and} \quad (10)$$

$$\int_a^b f(x) dx = \frac{h}{3} \left[f(x_0) + 2 \sum_{j=1}^{n/2-1} f(x_{2j}) + 4 \sum_{j=1}^{n/2} f(x_{2j-1}) + f(x_n) \right] - \sum_{k=2}^{\infty} \frac{4(k-1)h^{2k+1}}{3(2k+1)!} \sum_{j=1}^{n/2} f^{(2k)}(x_{2j-1}). \quad (11)$$

Equation (11) can be found in Scarborough [3], in expanded form stating the first three terms of the error sum.

At this point, we can explain the behavior of the composite Simpson's rule applied to $\int_0^1 \frac{4 dx}{1+x^2}$. The sum over j in the error term of (11) is in fact the midpoint rule applied to $f^{(2k)}(x)$. Since with $f(x) = \frac{4}{1+x^2}$, $f^{(4)}(x) = \frac{96(5x^4 - 10x^2 + 1)}{(1+x^2)^5}$ and $\int_0^1 f^{(4)}(x) dx = 0$, the order h^4 error term in the composite Simpson's rule goes to zero as n increases, and we are left with the error being order h^6 .

Going further In the process of explaining this result, we see that (9) can be rewritten (replacing $f(x)$ by $f^{(2i)}(x)$) as

$$\begin{aligned} 2h \sum_{j=1}^{n/2} f^{(2i)}(x_{2j-1}) &= \int_a^b f^{(2i)}(x) dx - \sum_{k=1}^{\infty} \frac{2h^{2k+1}}{(2k+1)!} \sum_{j=1}^{n/2} f^{(2(k+i))}(x_{2j-1}) \\ &= f^{(2i-1)}(b) - f^{(2i-1)}(a) \\ &\quad - \sum_{k=1}^{\infty} \frac{2h^{2k+1}}{(2k+1)!} \sum_{j=1}^{n/2} f^{(2(k+i))}(x_{2j-1}). \end{aligned}$$

Defining $[f^{(i)}]_a^b \equiv f^{(i)}(b) - f^{(i)}(a)$ and $F_i \equiv \sum_{j=1}^{n/2} f^{(2i)}(x_{2j-1})$, this says

$$2hF_i = [f^{(2i-1)}]_a^b - \sum_{k=1}^{\infty} \frac{2h^{2k+1}}{(2k+1)!} F_{i+k}. \quad (12)$$

Applying this result to each of the composite rules leads to error expansions in terms of the odd derivatives of the function. For the trapezoidal and midpoint rules we shall get the classic Euler-Maclaurin summation formulas, although this is a new derivation. An excellent summary of the classical derivation can be found in Steffensen [4].

Euler-Maclaurin summation formulas

Trapezoidal rule The error term for the composite trapezoidal rule from (10) can be written as

$$E = -2h \sum_{k=1}^{\infty} \frac{2kh^{2k}}{(2k+1)!} F_k.$$

Applying (12) to the $k=1$ term gives

$$E = -\frac{2^2}{2!} \frac{1}{2} \frac{1}{3} h^2 \left([f']_a^b - 2h \sum_{k=1}^{\infty} \frac{h^{2k}}{(2k+1)!} F_{k+1} \right) - 2h \sum_{k=2}^{\infty} \frac{2kh^{2k}}{(2k+1)!} F_k,$$

where the reason for the introduction of $2^2/2!$ will shortly become clear. If we let $c_1 = \frac{1}{2} \cdot \frac{1}{3}$ and shift the summation variable in the first sum down by one, we have

$$E = -\frac{2^2 c_1}{2!} h^2 [f']_a^b - 2h \sum_{k=2}^{\infty} \left(\frac{2k}{(2k+1)!} - \frac{2^2 c_1}{2!(2k-1)!} \right) h^{2k} F_k.$$

Applying (12) to the $k=2$ term with $c_2 = \frac{1}{2^3} \cdot \frac{2}{5} - \frac{4!}{2!3!} \cdot \frac{c_1}{2^2}$ leads to

$$E = -\frac{2^2 c_1}{2!} h^2 [f']_a^b - \frac{2^4 c_2}{4!} h^4 [f^{(3)}]_a^b - 2h \sum_{k=3}^{\infty} \left(\frac{2k}{(2k+1)!} - \frac{2^2 c_1}{2!(2k-1)!} - \frac{2^4 c_2}{4!(2k-3)!} \right) h^{2k} F_k.$$

Continuing this process leads to representing the error for the composite Trapezoidal rule as

$$E = -\sum_{k=1}^{\infty} \frac{(2h)^{2k} c_k}{(2k)!} [f^{(2k-1)}]_a^b,$$

where

$$c_k = \frac{1}{2^{2k-1}} \frac{k}{2k+1} - \sum_{j=1}^{k-1} \frac{(2k)! c_j}{2^{2(k-j)} (2j)! (2(k-j)+1)!},$$

and so

$$\int_a^b f(x) dx = h \left[f(x_0) + 2 \sum_{j=1}^{n/2-1} f(x_{2j}) + f(x_n) \right] - \sum_{k=1}^{\infty} \frac{(2h)^{2k} c_k}{(2k)!} [f^{(2k-1)}]_a^b. \quad (13)$$

By evaluation, we see that $c_1 = 1/6$, $c_2 = -1/30$, $c_3 = 1/42$, $c_4 = -1/30$, etc., and (13) appears to be the Euler-Maclaurin summation formula. It looks different from the more classical form because (10) has a step of $2h$ rather than the usual h , necessitating the $(2h)^{2k}$ term in the second sum of (13). A complete proof of this new derivation, however, requires a verification that $c_k = B_{2k}$ for all k .

Bernoulli numbers Bernoulli polynomials can be defined from a number of different starting points, including $B_n(x+1) - B_n(x) = nx^{n-1}$ and $B'_n(x) = nB_{n-1}(x)$, or $\frac{\tau e^{\tau x}}{e^\tau - 1} = \sum_{k=0}^{\infty} \frac{\tau^k}{k!} B_k(x)$. These lead to the relationship

$$B_n(x+h) = \sum_{k=0}^n \binom{n}{k} h^{n-k} B_k(x), \quad (14)$$

and, with $h = 1$, the classic definition of the Bernoulli polynomials as

$$B_0(x) = 1 \quad \text{and} \quad \sum_{k=0}^{n-1} \binom{n}{k} B_k(x) = nx^{n-1}. \quad (15)$$

The Bernoulli numbers B_k are simply the Bernoulli polynomials evaluated at $x = 0$. It is straightforward to show that $B_k(1-x) = (-1)^k B_k(x)$, $B_1(1) = B_1 + 1$, $B_k(1) = B_k$ for $k > 1$, and so $B_k = 0$ for $k = 3, 5, 7, \dots$. They can be uniquely defined using (15) with $x = 0$ as

$$B_0 = 1, \quad B_1 = -\frac{1}{2} \quad \text{and} \quad \sum_{k=0}^{n-1} \binom{n}{k} B_k = 0.$$

Choosing $n = 2k + 1$ leads to the explicit formula for the Bernoulli numbers of even order

$$B_{2k} = \frac{2k-1}{2(2k+1)} - \sum_{j=1}^{k-1} \frac{(2k)! B_{2j}}{(2j)!(2(k-j)+1)!}. \quad (16)$$

Unfortunately, this is not the same as the result in (13). To get this result requires the second kind Bernoulli numbers $B_n(1/2) = (2^{1-n} - 1)B_n$. With $h = 1/2$ and $x = 0$ in (14) we have the relationship

$$\sum_{k=0}^n \binom{n}{k} 2^{k-n} B_k = (2^{1-n} - 1)B_n,$$

which with $n = 2k + 1$ leads to

$$\begin{aligned}
B_{2k} &= \frac{-1}{2k+1} \sum_{j=0}^{2k-2} \binom{2k+1}{j} 2^{j-2k} B_j \\
&= \frac{-1}{2k+1} \left[2^{-2k} - (2k+1)2^{-2k} + \sum_{j=1}^{k-1} \frac{(2k+1)!B_{2j}}{2^{2(k-j)}(2j)!(2(k-j)+1)!} \right] \\
&= \frac{1}{2^{2k-1}} \frac{k}{2k+1} - \sum_{j=1}^{k-1} \frac{(2k)!B_{2j}}{2^{2(k-j)}(2j)!(2(k-j)+1)!},
\end{aligned}$$

which is the same as in (13) with $c_i = B_{2i}$, thus completing the proof.

Midpoint rule Exactly the same approach can be taken with the error term for the midpoint rule. The algebra is almost identical, and leads to

$$\int_a^b f(x) dx = 2h \sum_{j=1}^{n/2} f(x_{2j-1}) + \sum_{k=1}^{\infty} \frac{(2h)^{2k} d_k}{(2k)!} [f^{(2k-1)}]_a^b, \quad (17)$$

where

$$(2k+1)d_k = \frac{1}{2^{2k}} - \sum_{j=1}^{k-1} \binom{2k+1}{2j} \frac{d_j}{2^{2(k-j)}}.$$

We recognize this as the second Euler-Maclaurin summation formula if $d_k = -B_{2k}(1/2)$. We can verify this by returning to (14) and setting $x = h = 1/2$ and $m = 2k + 1$, so

$$B_{2k+1}(1) = B_{2k+1} = 0 = \sum_{j=0}^{2k+1} \binom{2k+1}{j} 2^{j-2k-1} B_j(1/2).$$

Since $B_j(1/2) = 0$ for $j = 1, 3, 5, \dots$ and $B_0(1/2) = 1$, this can be rewritten as

$$\frac{1}{2^{2k}} + \sum_{j=1}^{k-1} \binom{2k+1}{2j} \frac{B_{2j}(1/2)}{2^{2(k-j)}} + (2k+1)B_{2k}(1/2) = 0.$$

This is just (17) with $d_k = -B_{2k}(1/2)$, which completes the result.

Simpson's rule Finally, we can apply the same approach to the error for Simpson's rule, leading to

$$\int_a^b f(x) dx = \frac{h}{3} \left[f(x_0) + 2 \sum_{j=1}^{n/2-1} f(x_{2j}) + 4 \sum_{j=1}^{n/2} f(x_{2j-1}) + f(x_n) \right] + \sum_{k=1}^{\infty} \frac{h^{2k} e_k}{(2k)!} [f^{(2k-1)}]_a^b, \quad (18)$$

where

$$(2k+1)e_k = \frac{2(k-1)}{3} - \sum_{j=1}^{k-1} \binom{2k+1}{2j} e_k.$$

Note that $e_1 = 0$, and the first error term is of order h^4 as expected. After evaluating the first few e_i s, we see a pattern which suggests that $e_i = -\frac{4}{3}(4^{i-1} - 1)B_{2i}$. This can be proven by beginning with (16) and multiplying by $-4^{k-1}(2k+1)$, giving

$$-4^{k-1}(2k+1)B_{2k} = -\frac{k}{2} + \sum_{j=1}^{k-1} \binom{2k+1}{2j} 4^{j-1} B_{2j}. \quad (19)$$

Adding (19) to (16) multiplied by $(2k+1)$, then multiplying the sum by $4/3$ gives

$$(2k+1) \left[-\frac{4}{3}(4^{k-1} - 1)B_{2k} \right] = \frac{2(k-1)}{3} - \sum_{j=1}^{k-1} \binom{2k+1}{2j} \left[-\frac{4}{3}(4^{j-1} - 1)B_{2j} \right],$$

which is equivalent to (18) with the suggested relationship. Thus, an Euler-Maclaurin-like summation formula using Simpson's rule is

$$\int_a^b f(x) dx = \frac{h}{3} \left[f(x_0) + 2 \sum_{j=1}^{n/2-1} f(x_{2j}) + 4 \sum_{j=1}^{n/2} f(x_{2j-1}) + f(x_n) \right] - \frac{4}{3} \sum_{k=2}^{\infty} \frac{h^{2k}(4^{k-1} - 1)B_{2k}}{(2k)!} [f^{(2k-1)}]_a^b. \quad (20)$$

In principle, there is no reason why the same process cannot be applied to form Euler-Maclaurin-like formulas for other Newton-Cotes integration formulas. In fact, some of these formulas can be found in Uspensky [5], another paper whose contents have not been reproduced in undergraduate textbooks, despite the popularity and importance of the Euler-Maclaurin summation formula. However, Uspensky's derivation is far less straightforward than that presented here.

References

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