Lecture `quad2`: Numerical Quadrature: Error for Newton–Cotes

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Summary: Error analysis for the trapezoid and parabolic rules. Description of formula for general (closed) Newton–Cotes rule. Along the way, some motivation as to why error formulas are so useful.

References: Material here taken mostly from C. F. Van Loan's *Introduction to Scientific Computing*. See also T. Sauer's *Numerical Analysis*, Section 5.2, 1st ed. pages 253–263, 2nd ed. pages 254–265.

1 Comments

So long as we have the ability to evaluate $f(x)$ at the Newton–Cotes nodes, the quadrature formulas introduced last time can be used right "out of the box" to yield an approximation $Q_{NC(m)}$ to the definite integral

$$I = \int_a^b f(x)dx. \tag{1}$$

But how well does the value $Q_{NC(m)}$ agree with the value I? If I can be computed analytically, then we can check the answer. By *analytically*, we mean by an exact "pencil–and–paper" method, such as the Fundamental Theorem of Calculus (or perhaps Contour Integration in Complex Analysis). But that flys in the face of the motivation for numerical integration. We need to integrate functions which can **not** be integrated analytically. For these cases how do we know how accurate our answer is? Let's start by addressing this issue for the trapezoid rule $Q_{NC(2)}$, the simplest (closed) Newton–Cotes rule.

2 Error analysis of the trapezoid rule

Theorem 1. If $f(x)$ is twice continuously differentiable on an open interval which contains $[a, b]$, then

$$\left| \int_a^b f(x)dx - Q_{NC(2)} \right| \leq \frac{1}{12}(b-a)^3 M_2, \tag{2}$$

where $|f''(x)| \leq M_2$ for $x \in [a, b]$.

Before proving the theorem, let's first talk about what it says. Loosely speaking, it tells us that the trapezoid rule produces a good approximation to the definite integral whenever $b - a$ or the second derivative $f''(x)$ is small (or both). Whereas we may not be able to compute an antiderivative of $f(x)$ (that's why we're doing numerical quadrature in the first place!), we often **can** compute the second derivative $f''(x)$ and estimate M_2. For example, if $f(x) = \cos(x^2)$ (no elementary antiderivative!), then we straightforwardly find $f''(x) = -2\sin(x^2) - 4x^2\cos(x^2)$ and so $M_2 = 2 + 4b^2$ is a valid choice for the upper bound on $|f''(x)|$, provided $|b| > |a|$. Now we can make definitive statements like

$$\left| \int_0^{\frac{1}{10}} \cos(x^2)dx - Q_{NC(2)} \right| \leq \frac{1}{12}\frac{1}{10^3}\left(2 + \frac{4}{10^2}\right) \simeq 0.00017, \tag{3}$$

so the theorem indeed offers concrete knowledge. We expect that $Q_{NC(2)}$ is good to 3 digits past the decimal place. Indeed, with our script `ClosedQNC` (see last lecture) and with a MATLAB function `cosx2` for $\cos(x^2)$, we find

```
>> format long
>> ClosedQNC(@cosx2,0,1/10,2)
ans =
   0.099997500020833
```

Therefore, using the error estimate, we might report $I = 0.10000 \pm 0.00017$.

Proof of Theorem 1. We start by writing down the polynomial $q(x)$ which interpolates $f(x)$ at a, b, t, where t is a generic point on the interval. For the first part of the proof in this paragraph, we will obtain from $q(x)$ a key formula, whose integral will yield the result after some more work. In terms of Newton divided differences, the polynomial $q(x)$ has the form

$$\begin{aligned} q(x) &= f(a) + f[a,b](x-a) + f[a,b,t](x-a)(x-b) \\ &= p_1(x) + f[a,b,t](x-a)(x-b), \end{aligned} \tag{4}$$

where $p_1(x)$ is the unique degree–1 polynomial which interpolates $f(x)$ at $x = a, b$. If $t \in (a, b)$, that is $t \neq a$ and $t \neq b$, then $q(x)$ is a standard interpolating polynomial. However, if $t = b$, for example, then we adopt the intepretation $f[b, b] = f'(b)$. For this case

$$q(x) = f(a) + f[a,b](x-a) + \frac{f'(b) - f[a,b]}{b-a}(x-a)(x-b), \quad (\text{case } t = b), \tag{5}$$

so $q(x)$ is a *Hermite* interpolating polynomial obeying $q(a) = f(a), q(b) = f(b)$, and $q'(b) = f'(b)$. We obtain a similar Hermite interpolating polynomial if $t = a$, interpreting $f[a, a]$ as $f'(a)$. Recall that Hermite interpolation includes derivative information. Now, by construction $q(t) = f(t)$. Whence upon evaluating (4) at $x = t$ and then swapping t for x, we arrive at

$$f(x) = p_1(x) + f[a,b,x](x-a)(x-b). \tag{6}$$

Next, we use a basic fact about divided differences:

$$f[a,b,x] = \frac{1}{2} f''(\eta_x) \tag{7}$$

where the x–dependent number $\eta_x \equiv \eta(x) \in [a, b]$, a fact we'll demonstrate at the end. So far we've shown that

$$f(x) - p_1(x) = \frac{1}{2} f''(\eta_x)(x-a)(x-b), \tag{8}$$

which is our desired formula.

Let us now integrate (8), first noting that by the definition of the two–point closed Newton–Cotes rule (that is, the definition of the trapezoid rule)

$$Q_{NC(2)} = \int_a^b p_1(x)dx. \tag{9}$$

Therefore upon integration, (8) becomes

$$\int_a^b f(x)dx - Q_{NC(2)} = \frac{1}{2}\int_a^b f''(\eta_x)(x-a)(x-b)dx. \tag{10}$$

The appendix considers a more involved argument based on the last equation. Here we simply compute the following chain of estimates:

$$\begin{aligned}\left|\int_a^b f(x)dx - Q_{NC(2)}\right| &= \frac{1}{2}\left|\int_a^b f''(\eta_x)(x-a)(x-b)dx\right| \\ &\le \frac{1}{2}\int_a^b \big|f''(\eta_x)(x-a)(x-b)\big|dx \\ &\le \frac{1}{2}M_2\int_a^b \big|(x-a)(x-b)\big|dx. \qquad (11)\end{aligned}$$

Finally, noticing that $|(x-a)(x-b)| = (b-x)(x-a)$ on $[a,b]$, we then compute

$$\int_a^b (b-x)(x-a)dx = \frac{1}{6}(b-a)^3. \qquad (12)$$

We obtain (2) from this result and (11).

To complete our proof, we must show (7). To that end, define

$$h(x) \equiv f(x) - q(x). \qquad (13)$$

We consider three cases: (i) $t \in (a,b)$, in which case $h(x)$ vanishes at a, b, t; (ii) $t = a$, in which case $h(x)$ vanishes at a, b and $h'(a) = 0$; and (iii) $t = b$, in which case $h(x)$ vanishes at a, b and $h'(b) = 0$. For case (i), since $h(x)$ is continuously differentiable, by the Mean Value Theorem $h'(x)$ must have two roots, one on (a,t) and one on (t,b). Since $h'(x)$ has two roots and is itself continuously differentiable, another appeal to the Mean Value Theorem shows that $h''(x)$ has one root $\eta_t \equiv \eta(t)$ (it depends on the choice of t) between the two roots of $h'(x)$. Therefore, $h''(\eta_t) = 0$, or

$$f''(\eta_t) - q''(\eta_t) = 0 \iff f[a,b,t] = \frac{1}{2}f''(\eta_t), \qquad (14)$$

where (7) follows upon swapping the dummy variable t for x. Cases (ii) and (iii) are similar, and we only give details for (iii). In this case the Mean Value Theorem ensures that $h'(x)$ has one root on (a,b), but we already know that b is another root of $h'(x)$. So $h'(x)$ has two distinct roots. Another appeal the Mean Value Theorem then shows that $h''(x)$ vanishes at a point η_b on (a,b). Similarly, for case (ii) there exists an η_a for which $h''(\eta_a) = 0$. $\square$.

3 Error analysis of Simpson's Rule

Let's now turn the error formula for $Q_{NC(3)}$, whose proof follows similar lines to the one just considered. We'll not provide quite as much detail here.

Theorem 2. If $f(x)$ is four-times continuously differentiable on an open interval which contains $[a,b]$, then

$$\left|\int_a^b f(x)dx - Q_{NC(3)}\right| \le \frac{(b-a)^5}{2880}M_4, \qquad (15)$$

where $|f^{(4)}(x)| \le M_4$ for $x \in [a,b]$. **Important observation:** The error involves $(b-a)^5$ and a bound for $|f^{(4)}(x)|$, rather than $(b-a)^4$ and a bound for $|f^{(3)}(x)|$!

Proof of Theorem 2. We start with the polynomial that interpolates $f(x)$ at $a, b, c, d, t \in [a,b]$, here expressed in terms of Newton divided differences,

$$\begin{aligned}q(x) &= f(a) + f[a,b](x-a) + f[a,b,c](x-a)(x-b) \\ &\quad + f[a,b,c,d](x-a)(x-b)(x-c) + f[a,b,c,d,t](x-a)(x-b)(x-c)(x-d). \qquad (16)\end{aligned}$$

Later we choose $d = c$, and again t could be either a or b (or c); whence we are again using the Newton construction in a broader sense allowing for Hermite interpolation. At this point, relative to the proof of **Theorem 1** and (4), it may seem that we've made an error. In going from the proof of $Q_{NC(2)}$ to the one at hand for $Q_{NC(3)}$ ($m = 2$ to $m = 3$), we have added *two* term extra terms to $q(x)$. But we are not over–reaching! By construction $q(t) = f(t)$. Whence, evaluating the last equation at t and then swapping t for x, we obtain

$$\begin{aligned} f(x) = f(a) &+ f[a,b](x-a) + f[a,b,c](x-a)(x-b) \\ &+ f[a,b,c,d](x-a)(x-b)(x-c) + f[a,b,c,d,x](x-a)(x-b)(x-c)(x-d). \end{aligned} \tag{17}$$

Next we use a result similar to (7) for the higher order Newton divided difference (see Van Loan, page 90 for a proof)

$$f[a,b,c,d,x] = \frac{1}{24} f^{(4)}(\eta_x), \tag{18}$$

where $\eta_x \in [a,b]$. We now assume that $c = \frac{1}{2}(a+b)$ is the midpoint of the interval, so that

$$p_2(x) = f(a) + f[a,b](x-a) + f[a,b,c](x-a)(x-b) \tag{19}$$

$p_2(x)$ is the quadratic polynomial upon which Simpson's rule is based. Therefore, (17) becomes

$$f(x) - p_2(x) - f[a,b,c,d](x-a)(x-b)(x-c) = \frac{1}{24} f^{(4)}(\eta_x)(x-a)(x-b)(x-c)(x-d). \tag{20}$$

This is the formula we need.

Integration of (20) yields

$$\begin{aligned} &\int_a^b f(x)dx - Q_{NC(3)} - f[a,b,c,d] \int_a^b (x-a)(x-c)(x-b)dx = \\ &\qquad \frac{1}{24} \int_a^b f^{(4)}(\eta_x)(x-a)(x-b)(x-c)(x-d)dx. \end{aligned} \tag{21}$$

The polynomial $h(x) = (x-a)(x-c)(x-b)$ is odd about $x = c = \frac{1}{2}(a+b)$, by which we mean $h(c-t) = -h(c+t)$ (you should check this). But in the last equation $h(x)$ is being integrated over $[a,b]$, that is symmetrically about c. Whence this integral vanishes (that's the remarkable part of the proof). Now choosing $d = c$, we have the estimates

$$\begin{aligned} \left| \int_a^b f(x)dx - Q_{NC(3)} \right| &= \left| \frac{1}{24} \int_a^b f^{(4)}(\eta_x)(x-a)(x-b)(x-c)^2 dx \right| \\ &\le \frac{1}{24} \int_a^b \left| f^{(4)}(\eta_x)(x-a)(x-b)(x-c)^2 \right| dx \\ &\le \frac{1}{24} M_4 \int_a^b \left| (x-a)(x-b)(x-c)^2 \right| dx. \end{aligned} \tag{22}$$

Finally, on $[a,b]$ we have $|(x-a)(x-b)(x-c)^2| = (x-a)(b-x)(x-c)^2$, and (assuming c is the midpoint)

$$\int_a^b (x-a)(b-x)(x-c)^2 dx = \frac{1}{120}(b-a)^5, \tag{23}$$

which upon substitution into (22) proves the theorem.

4 Error formula for general closed Newton–Cotes rule

General Theorem. Suppose $f(x)$ possesses up to $d+1$ (d to be specified) derivatives which are continuous on $[a,b]$. Then (see Van Loan, page 142)

$$\left| \int_a^b f(x)dx - Q_{NC(m)} \right| \leq |c_m| M_{(d+1)} \left(\frac{b-a}{m-1} \right)^{d+2}, \qquad d = \begin{cases} m-1 & \text{if } m \text{ even} \\ m & \text{if } m \text{ odd,} \end{cases} \tag{24}$$

where M_{d+1} is a bound on $|f^{(d+1)}(x)|$ uniform over $x \in [a,b]$, and c_m is a constant (see list in Van Loan, page 142), for example,

$$c_2 = -\frac{1}{12}, \quad c_3 = -\frac{1}{90}, \quad c_4 = -\frac{3}{80}, \quad c_5 = -\frac{8}{945}, \quad c_6 = -\frac{275}{12096}. \tag{25}$$

The result indicates that $Q_{NC(4)}$ is not much better than $Q_{NC(3)}$, $Q_{NC(6)}$ not much better than $Q_{NC(5)}$, and so on. **Lesson:** use Newton–Cotes with an odd number of points. The negative signs are present on the c_m, because also (see the previous footnote)

$$\int_a^b f(x)dx - Q_{NC(m)} = c_m f^{(d+1)}(\eta) \left(\frac{b-a}{m-1} \right)^{d+2}, \tag{26}$$

with no absolute values, d as above, and unknown $\eta \in [a,b]$.

Appendix

This appendix takes a closer look at (10). On page 255 of the textbook, Sauer continues with this formula as follows. Since $f''(\eta_x) = f''(\eta(x)) = (f'' \circ \eta)(x)$ and $f''(x)$ is continuous by assumption, $f''(\eta_x)$ depends continuously on x if $\eta_x = \eta(x)$ does. Indeed, then $f''(\eta_x)$ is the composition of continuous functions. Since $(x-a)(b-x)$ is non-negative on $[a,b]$, we may then use the Integral Mean Value Theorem [cf. page 22 of the textbook] to conclude

$$\int_a^b f(x)dx - Q_{NC(2)} = -\frac{1}{2} f''(\eta) \int_a^b (x-a)(b-x)dx = -\frac{1}{12} f''(\eta) h^3,$$

where $\eta \in [a,b]$ is an unknown x-independent number (computation of which would be tantamount to analytical evaluation of the integral) and Sauer's $h = (b-a)$. This notation, and also Sauer's notation, is perhaps too compressed, since η in the last formula would be $\eta_c = \eta(c)$ for some fixed $c \in [a,b]$.

The argument above requires proof that η_x depends continuously on x. Here is an argument which does not use the Integral Mean Value Theorem *per se*. Since $\eta_x \in [a,b]$, we know $m \leq f''(\eta_x) \leq M$, where $m = \min_{a \leq x \leq b} f''(x)$ and $M = \max_{a \leq x \leq b} f''(x)$. These numbers exist because $f''(x)$ is continuous on $[a,b]$ by assumption. Then $m(x-a)(b-x) \leq f''(\eta_x)(x-a)(b-x) \leq M(x-a)(b-x)$, since $(x-a)(b-x) \geq 0$ for $x \in [a,b]$. Integration of the last inequality yields

$$\frac{1}{6} m(b-a)^3 \leq \int_a^b f''(\eta_x)(x-a)(x-b)dx \leq \frac{1}{6} M(b-a)^3.$$

But $\frac{1}{6} f''(x)(b-a)^3$ attains all values between $\frac{1}{6} m(b-a)^3$ and $\frac{1}{6} M(b-a)^3$ as x varies over $[a,b]$. So there exists at least one $\eta \in [a,b]$ such that

$$\frac{1}{6} f''(\eta)(b-a)^3 = \int_a^b f''(\eta_x)(x-a)(x-b)dx,$$

giving the above result without the assumption that η_x depends continuously on x.