Atlantic Electronic
Journal of Mathematics
Volume **5**, Number **1**, Winter **2012**

http://aejm.ca
http://aejm.ca/rema
pp. **47–59**

SIMPLE DERIVATION OF BASIC QUADRATURE FORMULAS

Erik Talvila

Department of Mathematics and Statistics
University of the Fraser Valley
Abbotsford, BC V2S 7M8

Matthew Wiersma

Department of Pure Mathematics
University of Waterloo
Waterloo, ON N2L 3G1

Abstract. Simple proofs of the midpoint, trapezoidal and Simpson's rules are proved for numerical integration on a compact interval. The integrand is assumed to be twice continuously differentiable for the midpoint and trapezoidal rules, and to be four times continuously differentiable for Simpson's rule. Errors are estimated in terms of the uniform norm of second or fourth derivatives of the integrand. The proof uses only integration by parts, applied to the second or fourth derivative of the integrand, multiplied by an appropriate polynomial or piecewise polynomial function. A corrected trapezoidal rule that includes the first derivative of the integrand at the endpoints of the integration interval is also proved in this manner, the coefficient in the error estimate being smaller than for the midpoint and trapezoidal rules. The proofs are suitable for presentation in a calculus or elementary numerical analysis class. Several student projects are suggested.

1. **Introduction.** Virtually every calculus text contains a section on numerical integration. Typically, the midpoint, trapezoidal and Simpson's rules are given. Derivation of these quadrature formulas are usually presented, often in a graphical manner, but most texts shy away from giving proofs of the error estimates. For example, according to [29], the book *Calculus*, by James Stewart, currently outsells all other calculus texts combined in North America. This astonishingly popular middle brow book gives error formulas for the midpoint, trapezoidal and Simpson's rules but provides no proofs [35]. In this paper we give simple proofs of these three basic quadrature rules and also a modified trapezoidal rule that includes first derivative terms and has a smaller error estimate than the usual midpoint and trapezoidal rules (Theorem 1). The proofs are based on integration by parts of $\int_a^b f''(x)p(x)\,dx$ or $\int_a^b f^{(4)}(x)p(x)\,dx$, where $\int_a^b f(x)\,dx$ is the integral the rule applies to and p is a polynomial or piecewise polynomial. Some elementary optimisation is also required. The proofs of these four rules are all easy enough for a standard calculus course.

2000 *Mathematics Subject Classification.* Primary: 26D15, 65D30; Secondary: 26A42, 41A55, 65D32.

Key words and phrases. Analytic inequalities, numerical integration.

The first author was supported by a Discovery Grant, the second author was supported by an Undergraduate Student Research Award; both from the Natural Sciences and Engineering Research Council of Canada. This paper was written while the first author was on leave and visiting the Department of Mathematical and Statistical Sciences, University of Alberta, and while the second author was a student at University of the Fraser Valley.

This paper will also be useful for a numerical analysis class. The proofs are self-contained except for an elementary lemma on polynomials (Lemma 1). We feel they are much simpler than methods usually employed in such courses. These often involve developing the theory of polynomial interpolation or special versions of the mean value theorem. Our proofs are constructive. For the midpoint and trapezoidal rules they begin with $\int_a^b f''(x)p(x)\,dx$, where p is a generic, monic quadratic or piecewise quadratic function. For Simpson's rule we begin with $\int_a^b f^{(4)}(x)p(x)\,dx$, where p is a monic, piecewise quartic function. After integration by parts it is clear what p has to be. For example, upon integrating by parts, one easily sees that the midpoint rule arises when $p(x) = (x-a)^2$ for $a \le x \le c$ and $p(x) = (x-b)^2$ for $c \le x \le b$. See Section 4. This makes it easy to produce new quadrature formulas. Our corrected trapezoidal rule, Theorem 1, is constructed so that the error is proportional to $(b-a)^3\|f''\|_\infty$ and the constant of proportionality is the smallest possible. The method we use appears in [18] and [7]. Both these sources give references to earlier practitioners of this method, such as Peano and von Mises.

In Section 6, we list a number of exercises, problems and projects. Some are at the calculus level but most are at the level of an undergraduate numerical analysis class.

We will consider numerical approximation of $\int_a^b f(x)\,dx$, under the assumption that f and its derivatives can be computed. For the midpoint and trapezoidal rules we assume $f \in C^2([a,b])$ (f and its derivatives to order 2 are continuous on interval $[a,b]$). For Simpson's rule we assume $f \in C^4([a,b])$. Error estimates will be obtained from integrals of the form $\int_a^b f^{(m)}(x)p(x)\,dx$ where p is a polynomial or piecewise polynomial and m is 2 or 4. Thus, all integrals that appear can be considered as Riemann integrals. In Section 6, projects 7, 8 and 14 discuss how assumptions on f can be weakened somewhat and then errors can be given in terms of Lebesgue or Henstock–Kurzweil integrals.

The usual midpoint, trapezoidal and Simpson's rules are as follows. Let n be a natural number. For $0 \le i \le n$ define $x_i = a + (b-a)i/n$. The midpoint of interval $[x_{i-1}, x_i]$ is $y_i = a + (b-a)(2i-1)/(2n)$. The symbol $\|f\|_\infty$ is the uniform norm of f and denotes the supremum of $|f(x)|$ for $x \in [a,b]$. If f is continuous then this is the maximum of $|f(x)|$.

Midpoint Rule. Let $f \in C^2([a,b])$. Write

$$\int_a^b f(x)\,dx = (b-a)f((a+b)/2) + E^M(f). \tag{1}$$

Then $|E^M(f)| \le (b-a)^3\|f''\|_\infty/24$. The composite midpoint rule is

$$\int_a^b f(x)\,dx = \frac{b-a}{n}\sum_{i=1}^n f(y_i) + E_n^M(f), \text{ with } |E_n^M(f)| \le \frac{(b-a)^3\|f''\|_\infty}{24n^2}.$$

Trapezoidal Rule. Let $f \in C^2([a,b])$. Write

$$\int_a^b f(x)\,dx = \frac{b-a}{2}\left[f(a) + f(b)\right] + E^T(f). \tag{2}$$

Then $|E^T(f)| \le (b-a)^3\|f''\|_\infty/12$. The composite trapezoidal rule is

$$\int_a^b f(x)\,dx = \frac{b-a}{2n}\left[f(a) + 2\sum_{i=1}^{n-1} f(x_i) + f(b)\right] + E_n^T(f), \text{ with } |E_n^T(f)| \le \frac{(b-a)^3\|f''\|_\infty}{12n^2}.$$

Simpson's Rule. Let $f \in C^4([a,b])$. Write

$$\int_a^b f(x)\,dx = \frac{b-a}{6}\left[f(a) + 4f((a+b)/2) + f(b)\right] + E^S(f). \tag{3}$$

Then $|E^S(f)| \le (b-a)^5 \|f^{(4)}\|_\infty/2880$. Let n be even. The composite Simpson's rule is

$$\int_a^b f(x)\,dx = \frac{b-a}{3n}\left[f(a) + 2\sum_{i=1}^{n/2-1} f(x_{2i}) + 4\sum_{i=1}^{n/2} f(x_{2i-1}) + f(b)\right] + E_n^S(f), \tag{4}$$

with $|E_n^S(f)| \le (b-a)^5\|f^{(4)}\|_\infty/(180n^4)$.

Many authors give the error for the trapezoidal rule as $E_n^T(f) = (b-a)^3 f''(\xi)/(12n^2)$, where ξ is some point in $[a,b]$. There are similar forms for the other rules. We don't find these any more useful than the uniform norm estimates. Unless we know something about f beyond continuity of its derivatives, it is impossible to say what ξ is.

Note that the approximation in Simpson's rule can be written

$$\int_a^b f(x)\,dx \doteq \frac{b-a}{3n}\left[f(a) + 4f(x_1) + 2f(x_2) + \cdots + 2f(x_{n-2}) + 4f(x_{n-1}) + f(b)\right].$$

Proofs of these three rules are given in Sections 4, 2 and 5, respectively.

The literature on these formulas is vast. Here is a sample of some of the different methods of proof that have been published in calculus texts. There are proofs based on the mean value theorem and Rolle's theorem [25], and polynomial interpolation [1]. Several authors produce a somewhat mystical auxiliary function and employ the mean value theorem or intermediate value theorem with integration by parts. For example, [20], [27]. All of the methods listed above appear in several sources.

There are many elementary journal articles that treat numerical integration. For a geometrical version of the midpoint rule, see Hammer [16]. Cruz-Uribe and Neugebauer [8] give a basic proof of the trapezoidal rule using integration by parts. Rozema [32] shows how to estimate the error for the trapezoidal rule, Simpson's rule and various versions of these rule that are corrected with derivative terms. Hart [17] also considers corrected versions of the trapezoidal rule. Talman [36] proves Simpson's rule by using an extended version of the mean value theorem for integrals. For other commentary on Simpson's rule, see [33] and [42].

For a numerical analysis course, integration of polynomial interpolation approximations is frequently used. See [6]. See [18] for proofs based on the difference calculus. For Taylor series, [40]. The elementary textbook [3] uses a rather complicated method with Taylor series and a weighted mean value theorem for integrals. For more sophisticated audiences, there are proofs based on the Euler–Maclaurin summation formula and the Peano kernel. See [9] and [22]. General references for numerical integration are [9], [13], [21], [23], [34], [41] and [43]. Several other methods can be found here.

2. **Trapezoidal rule.** For all of the quadrature formulas we derive, the error is estimated from the integral $\int_a^b f^{(m)}(x)p(x)\,dx$, where p is a suitable polynomial or piecewise polynomial function.

We first consider the trapezoidal rule. The estimate is then $\int_a^b f(x)\,dx \doteq (b-a)[f(a)+f(b)]/2$.

Proof. Write $p(x) = (x-\alpha)^2 + \beta$, where the constants α and β are to be determined. Assume $f \in C^2([a,b])$. Integrate by parts to get

$$\begin{aligned}\int_a^b f''(x)p(x)\,dx &= f'(b)p(b) - f'(a)p(a) - \int_a^b f'(x)p'(x)\,dx \\ &= f'(b)p(b) - f'(a)p(a) - f(b)p'(b) + f(a)p'(a) + \int_a^b f(x)p''(x)\,dx.\end{aligned}$$

Since $p'' = 2$ we can solve for $\int_a^b f(x)\,dx$,

$$\int_a^b f(x)\,dx = \frac{1}{2}\left[-f(a)p'(a) + f(b)p'(b) + f'(a)p(a) - f'(b)p(b)\right] + E(f), \tag{5}$$

where $E(f) = \frac{1}{2}\int_a^b f''(x)p(x)\,dx$. To get the trapezoidal rule we require $p(a) = p(b) = 0$ and $-p'(a) = p'(b) = b-a$. (Since we want the trapezoidal rule for all such f, the four variables $f(a)$, $f(b)$, $f'(a)$ and $f'(b)$ are linearly independent.) The solution of this overdetermined system is $\alpha = (a+b)/2$ and $\beta = -(b-a)^2/4$. The required quadratic is then $p(x) = [x-(a+b)/2]^2 - (b-a)^2/4$. Now we can estimate the error by

$$|E(f)| \le \frac{1}{2}\int_a^b |f''(x)p(x)|\,dx \le \frac{\|f''\|_\infty}{2}\int_a^b |p(x)|\,dx. \tag{6}$$

To evaluate the last integral, let $h = (b-a)/2$ and note that

$$\int_a^b |p(x)|\,dx = \int_{-h}^h |x^2 - h^2|\,dx = 2\int_0^h (h^2 - x^2)\,dx = 4h^3/3.$$

We then get $|E(f)| \le (b-a)^3\|f''\|_\infty/12$.

Now let $n \ge 2$ and use this estimate on each interval $[x_{i-1}, x_i]$ for $1 \le i \le n$. Let y_i be the midpoint of $[x_{i-1}, x_i]$. We define the piecewise quadratic function $P\colon[a,b] \to \mathbb{R}$ by $P(x) = (x-y_i)^2 - (b-a)^2/(4n^2)$ if $x \in [x_{i-1}, x_i]$ for some $1 \le i \le n$. Now we have P continuous on $[a,b]$ with $P(x_{i-1}) = P(x_i) = 0$, $P'(x_i-) = (b-a)/n$ and $P'(x_i+) = -(b-a)/n$. For the composite rule, (5) gives

$$\begin{aligned}\int_a^b f(x)\,dx &= \sum_{i=1}^n \int_{x_{i-1}}^{x_i} f(x)\,dx \doteq \frac{(b-a)}{2n}\sum_{i=1}^n [f(x_{i-1}) + f(x_i)] \\ &= \frac{(b-a)}{2n}\left\{f(a) + 2[f(x_1) + f(x_2) + \cdots + f(x_{n-1})] + f(b)\right\}.\end{aligned}$$

Let $\Delta x = (b-a)/n$. The error is

$$\begin{aligned}|E_n^T(f)| &= \frac{1}{2}\left|\sum_{i=1}^n \int_{x_{i-1}}^{x_i} f''(x)P(x)\,dx\right| \le \frac{\|f''\|_\infty}{2}\sum_{i=1}^n \int_{x_{i-1}}^{x_i}\left|(x-y_i)^2 - \left(\frac{\Delta x}{2}\right)^2\right|dx \\ &= \|f''\|_\infty \sum_{i=1}^n \int_0^{\Delta x/2}\left[\left(\frac{\Delta x}{2}\right)^2 - x^2\right]dx = \|f''\|_\infty \sum_{i=1}^n \frac{2}{3}\left(\frac{\Delta x}{2}\right)^3 = \frac{(b-a)^3\|f''\|_\infty}{12n^2}.\end{aligned}$$

□

We consider this to be a completely elementary derivation of the trapezoidal rule. The method is perfectly suitable for presenting in a calculus class or numerical analysis class.

Notice that $p(x) = (x-a)(x-b)$ so it is not necessary for f' to be continuous, provided $f'(x)(x-a)$ and $f'(x)(x-b)$ have limits as $x \to a^+$ and $x \to b^-$, respectively.

In this case, f'' will not be bounded so different methods will be needed to estimate $\int_a^b f''(x)p(x)\,dx$. See projects 8 and 13 in Section 6.

3. **Corrected trapezoidal rule.** Quadrature rules are often constructed so that they are exact for polynomials of a certain degree. For example, see [18, §5.10]. Here we do something different. We will minimise the coefficient in the error estimate. In (6), we have $|\int_a^b f''(x)p(x)\,dx| \leq \|f''\|_\infty \int_a^b |p(x)|\,dx$. This is a version of the Hölder inequality and it is a standard result of functional analysis that this is the best possible estimate over all such f and p. See, for example, [14, p. 184]. For more on this point, see project 9 in Section 6. This begs the question: What values of α and β will minimise $\int_a^b |p(x)|\,dx$? One of the requirements that we obtained the trapezoidal rule in the above calculation was that the coefficients of $f'(a)$ and $f'(b)$ vanish in (5). When we choose α and β to minimise $\int_a^b |p(x)|\,dx$ the resulting quadrature formula will have derivatives of f. But who cares? If we are assuming we can estimate f'' then surely we can include first derivative terms.

We first need a lemma about polynomials that can minimise $\int_a^b |p(x)|\,dx$.

Lemma 1. *Fix $k \geq 1$. Let $\mathcal{P}_k$ be the monic polynomials of degree k, with real coefficients. Let $I(p) = \int_a^b |p(x)|\,dx$. If $p \in \mathcal{P}_k$ minimises I then p has k real roots in $[a, b]$, counting multiplicities.*

Proof. If $k = 1$ evaluation of $\int_a^b |x-c|\,dx$ shows the minimum occurs when $c = (a+b)/2$. This can also be seen graphically.

Now assume $k \geq 2$. If I is minimised by $p \in \mathcal{P}_k$ and p has a root that is not real then write $p(x) = [(x-c)^2 + d^2]q(x)$ where $c, d \in \mathbb{R}$, $d > 0$ and $q \in \mathcal{P}_{k-2}$. Then

$$\int_a^b |p(x)|\,dx = \int_a^b (x-c)^2|q(x)|\,dx + d^2 \int_a^b |q(x)|\,dx > \int_a^b (x-c)^2|q(x)|\,dx,$$

contradicting the assumption that p minimises I. A minimising polynomial then has k real roots, counting multiplicities.

Now suppose $p \in \mathcal{P}_k$ minimises I and $p(a-c) = 0$ for some $c > 0$. Then $p(x) = (x-a+c)q(x)$ for some $q \in \mathcal{P}_{k-1}$. And,

$$\int_a^b |p(x)|\,dx = \int_a^b (x-a)|q(x)|\,dx + c\int_a^b |q(x)|\,dx > \int_a^b (x-a)|q(x)|\,dx,$$

contradicting the assumption that p minimises I. Hence, p cannot have any roots that are less than a. A similar argument shows p cannot have roots greater than b. □

Now we can prove the corrected trapezoidal rule.

Theorem 1 (Corrected trapezoidal rule)**.** *Let $f \in C^2([a, b])$. Write*

$$\int_a^b f(x)\,dx = \frac{b-a}{2}\,[f(a) + f(b)] + \frac{3(b-a)^2}{32}\,[f'(a) - f'(b)] + E^{CT}(f). \tag{7}$$

Then $|E^{CT}(f)| \leq (b-a)^3\|f''\|_\infty/32$. The composite corrected trapezoidal rule is

$$\int_a^b f(x)\,dx = \frac{b-a}{2n}\left[f(a) + 2\sum_{i=1}^{n-1} f(x_i) + f(b)\right] + \frac{3(b-a)^2}{32n^2}\,[f'(a) - f'(b)] + E_n^{CT}(f),$$

with $|E_n^{CT}(f)| \leq (b-a)^3\|f''\|_\infty/(32n^2)$.

Proof. As in the proof of the trapezoidal rule in Section 2, we are led to $\int_a^b |p(x)|\,dx$ for p a polynomial in $\mathcal{P}_2$. But this time, we choose p to minimise this integral. Due to the lemma, we can write $p(x) = (x-\alpha)^2 - \gamma^2$ where $a \leq \alpha - \gamma \leq \alpha + \gamma \leq b$. Then p has zeros at $\alpha \pm \gamma$, which are in $[a,b]$. Let $q(\alpha,\gamma) = \int_a^b |(x-\alpha)^2 - \gamma^2|\,dx = \int_{a-\alpha}^{b-\alpha} |x^2-\gamma^2|\,dx$. This must be minimised over the triangular region $Q = \{(x,y) \in \mathbb{R}^2 \mid a \leq x \leq b, 0 \leq y \leq \min(x-a, b-x)\}$. Differentiating the integral with respect to α, we have

$$\begin{aligned}
\partial q(\alpha,\gamma)/\partial\alpha &= |(a-\alpha)^2-\gamma^2| - |(b-\alpha)^2-\gamma^2| \\
&= a^2 - 2a\alpha - b^2 + 2b\alpha \\
&\quad \begin{cases} < 0, & \text{when } a \leq \alpha < (a+b)/2 \\ = 0, & \text{when } \alpha = (a+b)/2 \\ > 0, & \text{when } (a+b)/2 < \alpha \leq b. \end{cases}
\end{aligned}$$

Hence, for each allowed γ the minimum of q in Q occurs at $\alpha = (a+b)/2$. Now let $r(\gamma) = q((a+b)/2, \gamma) = 2\int_0^h |x^2-\gamma^2|\,dx$, where $h = (b-a)/2$. Differentiating under the integral sign, we have

$$\begin{aligned}
r'(\gamma) &= -4\gamma \int_0^h \operatorname{sgn}(x^2-\gamma^2)\,dx = -4\gamma\left(-\int_0^\gamma dx + \int_\gamma^h dx\right) \\
&= 8\gamma(\gamma - h/2) \quad \begin{cases} < 0, & \text{when } 0 < \gamma < h/2 \\ = 0, & \text{when } \gamma = 0 \text{ or } h/2 \\ > 0, & \text{when } h/2 < \gamma \leq h. \end{cases}
\end{aligned}$$

Hence, the minimum of r occurs at $\gamma = h/2 = (b-a)/4$. Now evaluate

$$\begin{aligned}
q((a+b)/2, h/2) &= 2\int_0^h |x^2 - h^2/4|\,dx \\
&= 2h^3\left(\int_0^{1/2} (1/4 - x^2)\,dx + \int_{1/2}^1 (x^2 - 1/4)\,dx\right) \\
&= h^3/2 = (b-a)^3/16.
\end{aligned}$$

The minimising polynomial is then $p(x) = (x-(a+b)/2)^2 - (b-a)^2/16$. Using (5) we have

$$\int_a^b f(x)\,dx = \frac{b-a}{2}\,[f(a)+f(b)] + \frac{3(b-a)^2}{32}\,[f'(a)-f'(b)] + E^{CT}(f), \tag{8}$$

where $|E^{CT}(f)| \leq (b-a)^3\|f''\|_\infty/32$.

For the composite corrected trapezoidal rule, apply the above rule on each interval $[x_{i-1}, x_i]$ for $1 \leq i \leq n$. This gives

$$\begin{aligned}
\int_a^b f(x)\,dx &\doteq \frac{(b-a)}{2n}\sum_{i=1}^n [f(x_{i-1}) + f(x_i)] + \frac{3(b-a)^2}{32n^2}\sum_{i=1}^n [f'(x_{i-1}) - f'(x_i)] \\
&= \frac{(b-a)}{2n}\left\{f(a) + 2[f(x_1) + f(x_2) + \cdots + f(x_{n-1})] + f(b)\right\} \\
&\quad + \frac{3(b-a)^2}{32n^2}\left[f'(a) - f'(b)\right].
\end{aligned} \tag{9}$$

Let $\alpha_i = (x_{i-1}+x_i)/2 = y_i$ and $\gamma_i = (x_i - x_{i-1})/4 = (b-a)/(4n)$. The error estimate is

$$|E^{CT}(f)| \leq \frac{\|f''\|_\infty}{2} \sum_{i=1}^{n} \int_{x_{i-1}}^{x_i} |(x-\alpha_i)^2 - \gamma_i^2|\, dx \leq \frac{(b-a)^3 \|f''\|_\infty}{32n^2}.$$

□

In a one-variable calculus class, the minimisation problem can be done as above but without using partial derivative notation. Differentiating under the integral sign with respect to α and γ is justified with the Lebesgue dominated convergence theorem since the derivative of the integrand exists except at one point. To avoid higher integration theory, it is easy enough to evaluate $\int_a^b |(x-\alpha)^2 - \gamma^2|\, dx$ before differentiating with respect to α and γ. But, as pointed out in project 8 of Section 6, the method used in the proof is useful for minimising with respect to the p-norm of f.

Notice that in the composite rule the sum of derivative terms telescopes. This means that in (9) only $f'(a)$ and $f'(b)$ appear. The composite trapezoidal, midpoint and corrected trapezoidal rule all have an error term proportional to $(b-a)^3\|f''\|_\infty/n^2$. The constant of proportionality is 1/12, 1/24 and 1/32, respectively. So with the composite corrected trapezoidal rule we have a smaller error estimate but are only required to add the additional two terms $3(b-a)^2[f'(a)-f'(b)]/(32n^2)$ to the composite trapezoidal rule. If n is reasonably large this is a negligible amount of additional work. If f' can be computed at a and b this becomes an attractive quadrature rule.

The corrected trapezoidal rule given in Theorem 1 is not the usual one that has traditionally appeared in the literature. For example, in Conte and De Boor [6], Davis and Rabinowitz [9], Dragomir, et al [12], Pečarič and Ujevič [28], and Squire [34], the coefficient is 1/12 in place of our 3/32 in (7). The error estimate $(b-a)^5\|f^{(4)}\|_\infty/720$ is obtained by polynomial interpolation by Conte and De Boor in [6] and with a two-point Taylor expansion by Davis and Rabinowitz in [9]. Dragomir, et al [12], use Grüss's inequality. In their Lemma 2, the error is given with $\|f''\|_\infty$ replaced by $\sup_{[a,b]} f'' - \inf_{[a,b]} f''$. Pečarič and Ujevič [28] give the error estimate as $\sqrt{3}(b-a)^3\|f''\|_\infty/54$ in their equation (3.3). This also appears in Dedič, et al [10]. Cerone and Dragomir [4] have coefficient 1/8 in their equation (3.64) in place of our 3/32 in (7). Their error estimate is $(b-a)^3\|f''\|_\infty/24$, obtained with integration by parts. Squire [34] gives a number of rules that use derivatives but does not provide any error estimates. It is shown in [39] that the coefficient 1/32 in Theorem 1 is the best possible.

4. **Midpoint rule.** Notice that with the composite trapezoidal rule, values of f were brought forth at discontinuities in the derivative of p. For the midpoint rule we will define p so that there is a discontinuity in p' at the midpoint $c = (a+b)/2$. Assume p is piecewise monic quadratic so that it is continuous on $[a,b]$ with p' continuous on $[a,c)$ and on $(c,b]$.

Proof. Integrating by parts twice,

$$\int_a^b f''(x)p(x)\, dx = \int_a^c f''(x)p(x)\, dx + \int_c^b f''(x)p(x)\, dx$$

$$= -f'(a)p(a) + f(a)p'(a) + f'(b)p(b) - f(b)p'(b) - f(c)[p'(c-) - p'(c+)] + 2\int_a^b f(x)\, dx.$$

For the midpoint rule we require $p(a) = p'(a) = p(b) = p'(b) = 0$ and $p'(c-) - p'(c+) = 2(b-a)$. This gives

$$p(x) = \begin{cases} (x-a)^2, & a \le x \le c \\ (x-b)^2, & c \le x \le b. \end{cases}$$

The error satisfies

$$|E^M(f)| \le \frac{\|f''\|_\infty}{2}\left(\int_a^c (x-a)^2\,dx + \int_c^b (x-b)^2\,dx\right) = \frac{\|f''\|_\infty (b-a)^3}{24}.$$

The composite rule follows as with the composite trapezoidal rule. Note that p and p' vanish at a and b. Define $P(x) = (x-x_{i-1})^2$ for $x_{i-1} \le x \le y_i$ and $P(x) = (x-x_i)^2$ for $y_i < x < x_i$ for $1 \le i \le n$. Then P and P' have discontinuities only at the midpoints y_i. Integrating by parts $\int_a^b f''(x)P(x)\,dx$ then gives the composite rule. □

Notice that $p(x) = (x-a)^2$ for $a \le x \le c$ and $p(x) = (x-b)^2$ for $c \le x \le b$. Hence, it is not necessary for f or f' to be continuous, provided $f'(x)(x-a)^2$ and $f(x)(x-a)$ have limits as $x \to a^+$. Similarly, as $x \to b^-$. In this case, f'' will not be bounded so different methods will be needed to estimate $\int_a^b f''(x)p(x)\,dx$. See projects 8 and 13 in Section 6.

Various versions of the midpoint rule are given in [5].

5. **Simpson's rule.** In Simpson's rule there are function evaluations at endpoints a, b and at midpoint c. As we saw with the midpoint rule, when we integrate $\int_a^b f^{(4)}(x)p(x)\,dx$, discontinuities in p and its derivatives at c lead to evaluations of f and its derivatives at c. Assume that p is a monic quartic polynomial on $[a,c)$ and on $(c,b]$. As we will now see, the requirement that $p \in C^2([a,b])$ determines the coefficients of $f(a)$, $f(b)$ and $f(c)$ in Simpson's rule. A brief explanation of this phenomenon appears in [30]. It is similar to the construction of the Green's function for ordinary differential equations.

Proof. Integrate by parts four times to get

$$\begin{aligned}\int_a^b f^{(4)}(x)p(x)\,dx &= -f'''(a)p(a) + f'''(c)\left[p(c-) - p(c+)\right] + f'''(b)p(b) + f''(a)p'(a)\\ &- f''(c)\left[p'(c-) - p'(c+)\right] - f''(b)p'(b) - f'(a)p''(a) + f'(c)\left[p''(c-) - p''(c+)\right] \qquad (10)\\ &+ f'(b)p''(b) + f(a)p'''(a) - f(c)\left[p'''(c-) - p'''(c+)\right] - f(b)p'''(b) + 24\int_a^b f(x)\,dx.\end{aligned}$$

For our quadrature rule to have no evaluations of derivatives of f we need $p(a) = p'(a) = p''(a) = p(b) = p'(b) = p''(b) = 0$. This means there are constants d_1 and d_2 such that

$$p(x) = \begin{cases} (x-a)^3(x+d_1), & a \le x \le c \\ (x-b)^3(x+d_2), & c \le x \le b. \end{cases}$$

Continuity of p at c requires $p(c-) = p(c+)$. From this it follows that $d_1 + d_2 = -(a+b)$. The derivative of p is

$$p'(x) = \begin{cases} (x-a)^2(4x+3d_1-a), & a \le x < c \\ (x-b)^2(4x+3d_2-b), & c < x \le b. \end{cases}$$

Continuity of p' at c requires $p'(c-) = p'(c+)$. From this it follows that $3(d_2 - d_1) = b - a$. Solving these two linear equations gives $d_1 = -(a+2b)/3$ and $d_2 = -(2a+b)/3$. We now have

$$p''(x) = \begin{cases} 4(x-a)(3x-2a-b), & a \le x < c \\ 4(x-b)(3x-a-2b), & c < x \le b. \end{cases}$$

This shows that $p''(c-) = p''(c+) = (b-a)^2$. So $p \in C^2([a,b])$. Now,

$$p'''(x) = \begin{cases} 4(6x-5a-b), & a \le x < c \\ 4(6x-a-5b), & c < x \le b. \end{cases}$$

And, $p'''(a) = -4(b-a)$, $p'''(b) = 4(b-a)$, $p'''(c-) - p'''(c+) = 16(b-a)$. From (10) we get the required approximation in (3).

The polynomial we are using is

$$p(x) = \begin{cases} (x-a)^3(x-a/3-2b/3), & a \le x \le c \\ (x-b)^3(x-2a/3-b/3), & c \le x \le b. \end{cases}$$

The error is then

$$|E^S(f)| = \frac{1}{24}\left|\int_a^b f^{(4)}(x)p(x)\,dx\right| \le \frac{\|f^{(4)}\|_\infty}{24}\int_a^b |p(x)|\,dx.$$

Note that $a/3+2b/3-(a+b)/2 = (b-a)/6 > 0$ and $2a/3+b/3-(a+b)/2 = (a-b)/6 < 0$. Therefore, $\int_a^b |p(x)|\,dx = \int_a^c (x-a)^3(a/3+2b/3-x)\,dx + \int_c^b (b-x)^3(x-2a/3-b/3)\,dx$. The transformation $x \mapsto a+b-x$ shows these last two integrals are equal. Hence,

$$\begin{aligned} \int_a^b |p(x)|\,dx &= 2\int_a^c (x-a)^3(a/3+2b/3-x)\,dx \\ &= -2\int_a^c (x-a)^4\,dx + \frac{4(b-a)}{3}\int_a^c (x-a)^3\,dx \\ &= (b-a)^5/120. \end{aligned}$$

This gives Simpson's rule.

For the composite rule it is traditional to take n even, divide $[a,b]$ into $n/2$ equal subintervals and apply Simpson's rule on each interval $[x_{2i-2}, x_{2i}]$ for $1 \le i \le n/2$. The approximation is then

$$\begin{aligned} \int_a^b f(x)\,dx &= \sum_{i=1}^{n/2}\int_{x_{2i-2}}^{x_{2i}} f(x)\,dx \doteq \frac{(b-a)}{3n}\sum_{i=1}^{n/2}[f(x_{2i-2}) + 4f(x_{2i-1}) + f(x_{2i})] \\ &= \frac{(b-a)}{3n}\left[f(a) + 2\sum_{i=1}^{n/2-1} f(x_{2i}) + 4\sum_{i=1}^{n/2} f(x_{2i-1}) + f(b)\right]. \end{aligned}$$

The error is computed as with the trapezoidal rule. □

Notice that $p(x) = O((x-a)^3)$ as $x \to a^+$. Hence, it is not necessary for f', f'' or f''' to be continuous, provided $f'''(x)(x-a)^3$, $f''(x)(x-a)^2$ and $f'(x)(x-a)$ have limits as $x \to a^+$. Similarly, as $x \to b^-$. In this case, $f^{(4)}$ will not be bounded so different methods will be needed to estimate $\int_a^b f^{(4)}(x)p(x)\,dx$. See projects 8 and 13 in Section 6.

Liu [26] uses integration by parts to prove a version of Simpson's rule for which $f \in C^n([a,b])$.

6. **Classroom projects.** The methods we have used to produce the midpoint rule, the trapezoidal rule, the corrected trapezoidal rule and Simpson's rule are: integration by parts, basic optimisation, and a simple fact about integrals of polynomials (Lemma 1). We have not needed any of the machinery mentioned in the Introduction that is often used in other proofs. This means our methods are well suited for use by students. We list below a number of topics that can be investigated in the classroom.

Some are at the level of a calculus course, others would make good assignments or projects in a beginning numerical analysis course. A few would be suitable for a senior undergraduate research project or perhaps an M.Sc. project.

1. First order error estimates. In all of the above rules it is assumed that f'' exists. What if $f \in C^1([a,b])$ but $f \notin C^2([a,b])$? For example, $f(x) = x^\alpha$ on $[0,1]$ if $1 < \alpha < 2$. Then we could still derive quadrature formulas by using one integration by parts on $\int_a^b f'(x)p(x)\,dx$. We can get the trapezoidal rule if p is a linear function. The error estimate is then $(b-a)^2\|f'\|_\infty/4$. See [2] for a geometric proof or [8] for an integration by parts proof. (The constant of proportionality is misprinted as $1/2$ in [8].) Taking p to be piecewise linear produces the midpoint rule with the same error. The paper [7] gives several different types of error estimates based on f' for the trapezoidal and Simpson rules.

2. Midpoint modifications. In the midpoint rule, what happens if we allow evaluation of f or f' at the endpoints and midpoint of $[a,b]$? How does the composite rule then compare with the trapezoidal rule and corrected trapezoidal rules?

3. Periodic functions. If f is periodic and we integrate over one period, how do the quadrature formulas simplify? Note that for a periodic function, application of the trapezoidal rule actually gives the corrected trapezoidal rule. A much deeper discussion can be found in [9].

4. Higher order error estimates. If $f \in C^n([a,b])$ and p is a monic polynomial of degree $k \geq n$ then integrate by parts on $\int_a^b f^{(n)}(x)p(x)\,dx$ to get other quadrature formulas. If p is a piecewise polynomial then f and its derivatives can be made to be evaluated at discontinuities in the derivatives of p. It is possible to make a systematic study of quadrature formulas obtained in this manner. In the corrected trapezoidal rule, the quadratic polynomial that minimised $\int_a^b |f''(x)p(x)|\,dx$ caused the f' terms to telescope away (9). This phenomenon can also be investigated for higher degree polynomials.

5. Linear combinations. It is well known that Simpson's rule can be obtained as a linear combination of trapezoidal rules or of midpoint and trapezoidal rules. Look for other such relationships amongst the various rules discussed above.

In Romberg integration, one takes a linear combination of trapezoidal rules with n and $2n$. This yields a quadrature formula with improved error estimate. This hierarchy is then repeated. See [9]. Does the integral form of the trapezoidal rule error show how to do this? Can this be done with the corrected trapezoidal rule?

6. Finite differences. If f was a special function defined by a definite integral or series depending on a parameter then it may not be feasible to compute f'. Similarly if f was given by experimental data. In such cases, we could approximate derivatives by finite differences, $f'(x) \doteq [f(x) - f(x+h)]/h$ if h is small. Do this for the composite corrected trapezoidal rule and compute the resulting error.

7. Relaxing conditions on f. For $|\int_a^b f''(x)p(x)\,dx| \leq \|f''\|_\infty \int_a^b |p(x)|\,dx$ it is not necessary that f'' be continuous. If we use the Lebesgue integral, the conditions on f can be weakened to f' being absolutely continuous such that f'' is essentially bounded.

This is the same as f' being Lipschitz continuous. Similar remarks apply for Simpson's rule and in 1. above. Under the assumption that f' is Lipschitz continuous, what do the error estimates for the trapezoidal, corrected trapezoidal and midpoint rules become? What Lipschitz condition could be used for Simpson's rule?

8. Using other Lebesgue norms to estimate the error. If $f'' \in L^r([a,b])$ then the Hölder inequality gives $|\int_a^b f''(x)p(x)\,dx| \leq \|f''\|_r\|p\|_s$, with $1/r + 1/s = 1$. The case $r = \infty, s = 1$ has already been used. The cases $1 \leq r < \infty$ could be investigated. The case $r = s = 2$ serves as a good warm up since the integral $\int_a^b |p(x)|^2\,dx$ can be evaluated explicitly. The minimising method from the proof of Theorem 1 can be used. Similarly with Simpson's rule and 1. above. See [39] for p-norm estimates for modified trapezoidal rules.

9. Equality in the corrected trapezoidal error. At the beginning of Section 3 we mentioned that $|\int_a^b f''(x)p(x)\,dx| \leq \|f''\|_\infty\|p\|_1$. Show that for each quadratic p there is a function $f \in C^1([a,b])$ such that f'' is piecewise constant and $\int_a^b |f''(x)p(x)|\,dx = \|f''\|_\infty\|p\|_1$. Show that for each $\epsilon > 0$ there is a function $g \in C^2([a,b])$ such that $|\int_a^b g''(x)p(x)\,dx| \geq \|g''\|_\infty\|p\|_1 - \epsilon$.

10. Geometric proofs. Sketch the piecewise polynomial functions used in derivation of all the above rules. Can you find a geometric proof of the choice of minimising polynomial in the corrected trapezoidal rule? What about for minimising polynomials of $\|p\|_s$? For example, Derek Lacoursiere has observed that if p is the monic quadratic that minimises $\|p\|_\infty$ then $p(a) = |p(c)| = p(b)$.

11. Non-uniform partitions. The composite rules are much simpler when the partition is uniform. But by taking non-uniform partitions we can get smaller error estimates. This will happen if smaller subintervals are taken where $|f''|$ is large and larger subintervals are allowed where $|f''|$ is small. This could be done in a systematic way if, say, f'' was positive and decreasing. This opens up the creation of adaptive algorithms. See [41, p. 160] for a meta algorithm on adaptive integration. A basic example of such an algorithm is given in [3]. Rice [31] has estimated there "are from are from 1 to 10 million algorithms that are potentially interesting and significantly different from one another". Get cracking!

12. Error estimates on each subinterval. By taking properties of f into account it is possible to get better error estimates. Denote the characteristic function of interval $[s,t]$ by $\chi_{[s,t]}(x)$ and this is 1 if $x \in [s,t]$ and 0, otherwise. The estimate $\|f''\chi_{[x_{i-1},x_i]}\|_\infty \leq \|f''\|_\infty$ was used in the proof of the trapezoidal rule. (Can you see where?) It is the best we can do for generic f such that f'' is bounded, since then the supremum of $|f''|$ can occur on any subinterval. It may be fine if $f''(x) = \sin(1/x)$ on $[0,1]$ but is a poor estimate for $f(x) = \sqrt{x}$. If f'' was positive and increasing then $\|f''\chi_{[x_{i-1},x_i]}\|_\infty = f''(x_i) < \|f''\|_\infty$. This estimate can then be used on each subinterval. Similarly if f is decreasing.

13. Unbounded integrands. It is not necessary for f' or f'' to be integrable. If not, we may be able to integrate against a polynomial with a zero of sufficient multiplicity. For example, suppose $f \in C^2((0,1])$ such that $\int_0^1 f(x)\,dx$ exists and as $x \to 0^+$ we have $f(x) = o(1/x)$ and $f'(x) = o(1/x^2)$. An example of such a function on $[0, 1/2]$ is $f(x) = |\log x|^\alpha$ for each real α. Let $p(x) = x^2$. Then $\int_0^1 f''(x)p(x)\,dx = f'(1) - 2f(1) + 2\int_0^1 f(x)\,dx$. (This is Taylor's theorem.) Show this leads to a quadrature formula with error a multiple of $|\int_0^1 f''(x)x^2\,dx|$. If also $f''(x) = O(1/x^2)$ as $x \to 0^+$ then this integral is bounded by $\sup_{x\in[0,1]} |f''(x)x^2|$. There are similar results when $f(x) \sim c_1/x$ for some constant c_1 and $f'(x) \sim c_2/x^2$ for some constant c_2. It is easy to modify this for higher order singularities.

14. The Henstock–Kurzweil integral. The error estimates all depend on existence of $\int_a^b f''(x)p(x)\,dx$. There are functions that are differentiable at each point for which the derivative is not integrable in the Riemann or Lebesgue sense. An example is given by taking $g: [0, 1] \to \mathbb{R}$ as $g(x) = x^2 \sin(x^{-3})$ for $x > 0$ and $g(0) = 0$. Then g' exists at each point of $[0, 1]$ but is not continuous at 0. Since the derivative is not bounded, $\int_0^1 g'(x)\,dx$ does not exist as a Riemann integral. Since $\int_0^1 |g'(x)|\,dx = \infty$, we have $g' \notin L^1([0, 1])$. In this case, $\int_0^1 g'(x)\,dx$ exists as an improper Riemann integral. However, a construction in [19] shows how to use a Cantor set to piece together such functions so that improper Riemann integrals do not exist but the Henstock–Kurzweil integral exists.

The Henstock–Kurzweil integral is defined in terms of Riemann sums that are chosen somewhat more carefully than in Riemann integration. It has the property that if g' exists then $\int_a^b g'(x)\,dx = g(b) - g(a)$. In fact, if g is continuous, this fundamental theorem of calculus formula will still hold when g' fails to exist on countable sets and certain sets of measure zero. See [15]. Conditionally convergent integrals such as $\int_0^\infty x^2 \sin(e^x)\,dx$ also exist in this sense. With the Henstock–Kurzweil integral there is the estimate $|\int_a^b f(x)g(x)\,dx| \le \|f\|\|g\|_{\mathcal{BV}}$. The Alexiewicz norm of f is $\|f\| = \sup_{[c,d]\subset[a,b]} |\int_c^d f(x)\,dx|$. The function g must be of bounded variation and $\|g\|_{\mathcal{BV}} = \|g\|_\infty + Vg$, where Vg is the variation of g. See [24].

The conditions on f can then be relaxed to f'' integrable in the Henstock–Kurzweil sense and we can estimate $\int_a^b f''(x)p(x)\,dx$ using the Alexiewicz norm $\|f''\|$. See [11] and [39]. In fact, f'' need not even be a function. The same estimates hold when f' is merely continuous and then f'' exists in the distributional sense. See [37]. Similarly if f' has jump discontinuities of finite magnitude. See [38].

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Received September 2, 2011; revised December 31, 2011.

E-mail address: `erik.talvila@ufv.ca; mwiersma@uwaterloo.ca`