

OPTIMAL ERROR ESTIMATES FOR CORRECTED TRAPEZOIDAL RULES

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Abstract. Corrected trapezoidal rules are proved for $\int_a^b f(x) dx$ under the assumption that $f'' \in L^p([a, b])$ for some $1 \leq p \leq \infty$. Such quadrature rules involve the trapezoidal rule modified by the addition of a term $k[f'(a) - f'(b)]$. The coefficient k in the quadrature formula is found that minimizes the error estimates. It is shown that when f' is merely assumed to be continuous then the optimal rule is the trapezoidal rule itself. In this case error estimates are in terms of the Alexiewicz norm. This includes the case when f'' is integrable in the Henstock–Kurzweil sense or as a distribution. All error estimates are shown to be sharp for the given assumptions on f'' . It is shown how to make these formulas exact for all cubic polynomials f . Composite formulas are computed for uniform partitions.

1. Introduction

This paper is concerned with numerical integration schemes for $\int_a^b f(x) dx$ where it is assumed f' is absolutely continuous such that $f'' \in L^p([a, b])$ for some $1 \leq p \leq \infty$, or that f'' is integrable in the Henstock–Kurzweil sense, or that f' is continuous so that f'' exists as a distribution and is integrable using a distributional integral. Integration by parts shows that

$$\int_a^b f(x) dx = \frac{1}{2} [-f(a)\phi'(a) + f(b)\phi'(b) + f'(a)\phi(a) - f'(b)\phi(b)] + E(f), \quad (1.1)$$

where $E(f) = (1/2) \int_a^b f''(x)\phi(x) dx$ and ϕ is a monic quadratic polynomial. Observe that taking $\phi(x) = (x-a)(x-b)$ gives the usual trapezoidal rule $\int_a^b f(x) dx = (b-a)[f(a) + f(b)]/2 + E^T(f)$, where $E^T(f) = (1/2) \int_a^b f''(x)(x-a)(x-b) dx$. The Hölder inequality then gives $|E^T(f)| \leq \|f''\|_p \|\phi\|_q / 2$, where q is the conjugate exponent of p . Hence,

$$|E^T(f)| \leq \begin{cases} \|f''\|_1 (b-a)^2 / 8, & p = 1 \\ [B(q+1, q+1)]^{1/q} \|f''\|_p (b-a)^{2+1/q} / 2, & 1 < p < \infty \\ \|f''\|_\infty (b-a)^3 / 12, & p = \infty. \end{cases} \quad (1.2)$$

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Here, $B(x, y) = \Gamma(x)\Gamma(y)/\Gamma(x+y)$ is the beta function. See [4, Theorem 3.22]. (This corrects a typographical error in [4].)

We find ϕ that minimizes the error in (1.1). This leads to a quadrature rule that includes values of f and f' at the endpoints a and b . The error-minimizing polynomial produces the classical trapezoidal rule, modified by the addition of first derivative terms. In the literature this is called a corrected trapezoidal rule. This includes solving the problem of choosing $k \in \mathbb{R}$ to minimize all quadrature rules of the form $(b-a)[f(a)+f(b)]/2+k[f'(a)-f'(b)]$. The error terms are as in (1.2) but with the coefficient of $\|f''\|_p(b-a)^{2+1/q}$ minimized. In particular, the coefficients are strictly less than in (1.2). We prove our results are the best possible given the assumption $f'' \in L^p([a, b])$ (Theorem 2.1 and Corollaries 2.2-2.5). The composite formula (Corollary 2.5) provides an improved error estimate over the trapezoidal rule. Since the f' terms telescope, the correction terms only require computation of f' at endpoints a and b rather than at interior nodes. Compared to the usual trapezoidal rule the extra computing time to implement our corrected rule is then negligible for large n .

Finding the polynomial ϕ that minimizes the error in (1.1) involves solving a transcendental equation for a parameter in the polynomial. This transcendental equation is written in various ways in Section 3. When q is an integer this reduces to a polynomial equation for the parameter. We are able to solve for the exact value of the parameter when $p = 1, 2, 4/3, \infty$. See Corollaries 2.2-2.4 and (3.3). Even without knowing the parameter exactly, Theorem 3.2 gives a corrected trapezoidal rule with error estimate smaller than in (1.2).

In Section 5 we reduce the assumption on f to $f \in C^1([a, b])$ and then f'' exists as a distribution and is integrable using the continuous primitive integral (Corollary 5.3). This includes the case when f'' is integrable in the Henstock–Kurzweil sense (Theorem 5.1). The error estimate is then in terms of the Alexiewicz norm of f'' . In this case, the optimum form of (1.1) is the trapezoidal rule itself.

In Section 6 we compute ϕ so that (1.1) is exact for all cubic polynomials f . The required ϕ is the same as the one that minimizes the error in the case when $f'' \in L^2([a, b])$.

Several authors have considered corrected trapezoidal rules under the assumption that the derivatives of f are in various function spaces. See [4] (L^p), [8] (L^∞), [9] (Lipschitz, continuous and bounded variation, L^p), [10] (L^p , Henstock–Kurzweil integrable), [14] (continuous and bounded variation) and [17] (L^p).

2. Main theorem

The error in (1.1) is minimized over all monic polynomials ϕ . Results in Lemma 4.1 show that a unique error-minimizing polynomial exists and is of the form $\phi(x) = (x-c)^2 - \alpha^2$ such that c is the midpoint of $[a, b]$ and ϕ has two real roots in $[a, b]$. Note that (1.1) becomes a corrected trapezoidal rule precisely when $\phi'(b) = -\phi'(a) = b-a$ and this relation holds for $\phi(x) = (x-c)^2 - \alpha^2$. For a uniform partition the composite rule obtained from (1.1) will in general have f' evaluated at all points at which f is evaluated. However, when $\phi'(a) = \phi'(b)$ the sum of f' terms telescopes, leaving only

$f'(a)$ and $f'(b)$ (Corollary 2.5). This is the case with all the error-minimizing rules we present.

We are able to compute exact values for α when $p = 1, 2, 4/3, \infty$. In other cases α is given by the transcendental equation (2.10). When q is an integer this reduces to finding the largest real root of a polynomial of degree $2q - 1$.

THEOREM 2.1. *Let c be the midpoint of $[a, b]$. Let $f: [a, b] \rightarrow \mathbb{R}$ such that f' is absolutely continuous and $f'' \in L^p([a, b])$ for some $1 < p < \infty$. Let $1/p + 1/q = 1$. Amongst all monic quadratic polynomials used to generate (1.1), taking $\phi(x) = (x - c)^2 - \alpha_q^2$ gives the unique minimum for the error $|E(f)|$. The constant $\beta_q > 1$ is the unique solution of the equation*

$$\int_1^{\beta_q} (x^2 - 1)^{q-1} dx = \frac{1}{2} B(q, 1/2) = 2^{2q-2} B(q, q) \quad (2.1)$$

and $\alpha_q \beta_q = (b - a)/2$. This gives the quadrature formula

$$\int_a^b f(x) dx = \frac{b-a}{2} [f(a) + f(b)] + \frac{(b-a)^2}{8} (1 - \beta_q^{-2}) [f'(a) - f'(b)] + E(f), \quad (2.2)$$

where

$$|E(f)| \leq \frac{\|f''\|_p (b-a)^{2+1/q} (1 - \beta_q^{-2})}{2^{3+1/q} (q + 1/2)^{1/q}}. \quad (2.3)$$

The coefficient of $\|f''\|_p$ in the error bound is the best possible.

Note that the numbers α_q and β_q are independent of f , while β_q are also independent of the interval $[a, b]$.

COROLLARY 2.2. *If $p = 1$ and $q = \infty$ then $\beta_\infty = \sqrt{2}$, $\alpha_\infty = (b-a)/(2\sqrt{2})$ gives the unique minimum error. The quadrature formula is*

$$\int_a^b f(x) dx = \frac{(b-a)}{2} [f(a) + f(b)] + \frac{(b-a)^2}{16} [f'(a) - f'(b)] + E(f), \quad (2.4)$$

where the optimal error is $|E(f)| \leq \|f''\|_1 (b-a)^2/16$.

COROLLARY 2.3. *If $p = q = 2$ then $\beta_2 = \sqrt{3}$, $\alpha_2 = (b-a)/(2\sqrt{3})$ gives the unique minimum error. The quadrature formula is*

$$\int_a^b f(x) dx = \frac{(b-a)}{2} [f(a) + f(b)] + \frac{(b-a)^2}{12} [f'(a) - f'(b)] + E(f), \quad (2.5)$$

where the optimal error is $|E(f)| \leq \|f''\|_2 (b-a)^{2.5}/(12\sqrt{5})$.

COROLLARY 2.4. *If $p = \infty$ and $q = 1$ then $\beta_1 = 2$, $\alpha_1 = (b-a)/4$ gives the unique minimum error. The quadrature formula is*

$$\int_a^b f(x) dx = \frac{(b-a)}{2} [f(a) + f(b)] + \frac{3(b-a)^2}{32} [f'(a) - f'(b)] + E(f), \quad (2.6)$$

where the optimal error is $|E(f)| \leq \|f''\|_\infty (b-a)^3/32$.

Other authors have obtained corrected trapezoidal rules under the assumption $f'' \in L^p([a, b])$, generally with different coefficients of $f'(a) - f'(b)$ in (2.2) and strictly larger coefficients of $\|f''\|_p(b-a)^{2+1/q}$ than in (2.3). See Cerone and Dragomir [4] equation (3.64), where the coefficient of $f'(a) - f'(b)$ is $(b-a)^2/8$ for all values of p . In Theorem 3.24 for $p = \infty$ they have the coefficient of $f'(a) - f'(b)$ as $(b-a)^2/12$. This coefficient is only sharp for $p = 2$ (Corollary 2.3). The estimate $|E(f)| \leq [\sup(f) - \inf(f)](b-a)^3/(24\sqrt{5})$ is proved. Dedić, Matić and Pečarić [9, Corollaries 9, 12] also consider corrected trapezoidal rules with $f'' \in L^p([a, b])$. In their Corollary 9 they have the coefficient of $f'(a) - f'(b)$ as $(b-a)^2/12$ and prove the larger estimate $|E(f)| \leq \|f''\|_\infty(b-a)^3/(18\sqrt{3})$. The results of our Corollary 2.3 appear as their Corollary 12 (without sharpness). Similarly in [10].

COROLLARY 2.5. *For a uniform partition given by $x_i = a + (b-a)i/n, 0 \leq i \leq n$, the composite formula is*

$$\int_a^b f(x) dx = \frac{b-a}{2n} \left[f(a) + 2 \sum_{i=1}^{n-1} f(x_i) + f(b) \right] + \frac{(b-a)^2}{8n^2} (1 - \beta_q^{-2}) [f'(a) - f'(b)] + E(f), \tag{2.7}$$

where

$$|E(f)| \leq \begin{cases} \|f''\|_1(b-a)^2/(16n^2), & p = 1 \\ \frac{\|f''\|_p(b-a)^{2+1/q}(1-\beta_q^{-2})}{2^{3+1/q}(q+1/2)^{1/q}n^2}, & 1 < p < \infty \\ \|f''\|_\infty(b-a)^3/(32n^2), & p = \infty. \end{cases}$$

The coefficient of $\|f''\|_p$ in the error bound is the best possible.

Proof of Theorem 2.1. Let ϕ be a monic quadratic polynomial. Integration by parts gives (1.1). We are then led to minimize $E(f) = (1/2) \int_a^b f''(x)\phi(x) dx$. By the Hölder inequality, $|E(f)| \leq (1/2)\|f''\|_p\|\phi\|_q$. First consider a symmetric interval $[-a, a]$. By Lemma 4.1, to minimize $\|\phi\|_q$ we need only consider $\phi(x) = x^2 - \alpha^2$ for some $\alpha \in [0, a]$. Let $\beta = a/\alpha$. Define

$$G_q(\alpha) = \|\phi\|_q^q = 2 \int_0^a |x^2 - \alpha^2|^q dx = 2\alpha^{2q+1} \left(\int_0^1 (1-x^2)^q dx + \int_1^{a/\alpha} (x^2-1)^q dx \right). \tag{2.8}$$

Note that

$$G'_q(\alpha) = 4q\alpha^{2q} \left(\int_0^1 (1-x^2)^{q-1} dx - \int_1^{a/\alpha} (x^2-1)^{q-1} dx \right). \tag{2.9}$$

We have $G'_q(0) = 0$. Since the function $\alpha \mapsto \int_1^{a/\alpha} (x^2-1)^{q-1} dx$ decreases from positive infinity to zero as α increases from zero to a , it follows that G'_q has a unique root in $(0, a)$ and G_q has a unique minimum at $\alpha_q \in (0, a)$. The first integral in (2.9) can be evaluated in terms of beta and gamma functions. We have [16, 5.12.1]

$$\int_0^1 (1-x^2)^{q-1} dx = \frac{1}{2}B(q, 1/2) = 2^{2q-2}B(q, q) = \frac{\sqrt{\pi}\Gamma(q)}{2\Gamma(q+1/2)}.$$

Let $\beta_q = a/\alpha_q$. The required minimizing polynomial is then determined by the unique root $\beta_q \in (1, \infty)$ of the equation

$$\int_1^{\beta_q} (x^2 - 1)^{q-1} dx = \frac{1}{2} B(q, 1/2). \quad (2.10)$$

To compute $\|\phi\|_q$, evaluate the final integral in (2.8). Integration by parts establishes the recurrence relation

$$\int (x^2 - 1)^q dx = \frac{x(x^2 - 1)^q}{2q + 1} - \frac{2q}{2q + 1} \int (x^2 - 1)^{q-1} dx. \quad (2.11)$$

Using this and the corresponding version with integrand $(1 - x^2)^q$, we obtain $G_q(\alpha_q) = 2a(a^2 - \alpha_q^2)^q / (2q + 1)$. It then follows that

$$|E(f)| \leq \frac{\|f''\|_p (2a)^{2+1/q} [1 - (\alpha_q/a)^2]}{2^{3+1/q} (q+1/2)^{1/q}}.$$

Replacing a with $(b-a)/2$ establishes the error estimate for interval $[a, b]$. Using $\phi(x) = (x-c)^2 - \alpha_q^2$ the formula (2.2) now follows.

With the Hölder inequality, $|\int_a^b f''(x)\phi(x) dx| \leq \|f''\|_p \|\phi\|_q$, the necessary and sufficient condition for equality is $f''(x) = d \operatorname{sgn}[\phi(x)] |\phi(x)|^{1/(p-1)}$ for some $d \in \mathbb{R}$ and almost all $x \in [a, b]$. See [13, p. 46]. Integrating gives

$$f(x) = d \int_a^x (x-t) \operatorname{sgn}[\phi(t)] |\phi(t)|^{1/(p-1)} dt,$$

modulo a linear function. \square

Proof of Corollary 2.2. It suffices to consider the interval $[-a, a]$. When $p = 1$ write $\phi(x) = x^2 - \alpha_\infty^2$. By Lemma 4.1 we need only consider the case with two distinct roots in $(-a, a)$, i.e., $0 < \alpha_\infty < a$. We have

$$F_\infty(\phi) := \|\phi\|_\infty = \max_{|x| \leq a} |\phi(x)| = \max(|\phi(0)|, \phi(a)) = \max(\alpha_\infty^2, a^2 - \alpha_\infty^2).$$

It follows that $\alpha_\infty = a/\sqrt{2}$. Formula (2.4) and the error estimate now follow easily. There is equality in $|\int_{-a}^a f''(x)\phi(x) dx| \leq \|f''\|_1 \|\phi\|_\infty$ whenever $\phi(x) = d \operatorname{sgn}[f''(x)]$ for some $d \in \mathbb{R}$ and almost all $x \in [-a, a]$. See [13, p. 46]. This does not hold but we can show the coefficient of $\|f''\|_1$ cannot be reduced by considering a sequence of functions. If $f'' = \delta$, the Dirac distribution supported at 0, then $|\int_{-a}^a f''(x)(x^2 - \alpha_\infty^2) dx| = \alpha_\infty^2 = a^2/2 = \|f''\|_1 \|\phi\|_\infty$. Of course, if $f'' = \delta$ then $f' = \chi_{(0, \infty)}$ which is not absolutely continuous. Let (ψ_n) be a delta sequence. This is a sequence of continuous functions $\psi_n \geq 0$ with support in $(0, 1/n)$ such that $\int_0^{1/n} \psi_n(x) dx = 1$. Now define $f_n(x) = \int_{-a}^x \int_{-a}^y \psi_n(z) dz dy$. Then f_n' is absolutely continuous and $\|f_n''\|_1 = 1$. Since ϕ is continuous we have $\lim_{n \rightarrow \infty} |\int_{-a}^a f_n''(x)(x^2 - \alpha_\infty^2) dx| = a^2/2 = \|\phi\|_\infty$. The error estimate is then optimal. \square

Proof of Corollary 2.4. Write $\phi(x) = x^2 - \alpha_1^2$. By Lemma 4.1 we need only consider the case with two distinct roots in $(-a, a)$, i.e., $0 < \alpha_1 < a$. Equation (2.9) now becomes $G'_1(\alpha_1) = 2\alpha_1(12\alpha_1 - 6a)/3$, from which $\alpha_1 = a/2$. This then gives (2.6). There is equality in $|\int_{-a}^a f''(x)\phi(x)dx| \leq \|f''\|_\infty \|\phi\|_1$ whenever $f''(x) = d \operatorname{sgn}[\phi(x)]$ for some $d \in \mathbb{R}$ and almost all $x \in [-a, a]$. See [13, p. 46]. Integrating gives $f(x) = d \int_{-a}^x (x-t)\operatorname{sgn}[\phi(t)] dt$, modulo a linear function. \square

This case also appears in [22, Theorem 1].

The proof of Corollary 2.5 follows using the Hölder inequality for series as in the proof of Theorem 3.26 in [4].

Lemma 4.1 shows that the minimum of $\|\phi\|_q$ over monic quadratics is unique. Hence, the coefficient of $\|f''\|_p(b-a)^{2+1/q}$ in (2.3) is strictly less than for any other choice of α_q and indeed for any other choice of monic quadratic. In particular, we get a smaller coefficient than in the trapezoidal rule (1.2).

3. Evaluation and approximation of β_q

In Corollaries 2.2 through 2.4 we were able to compute the exact value of α_q and β_q for $q = 1, 2, \infty$. In this section we compute β_4 as the root of a cubic polynomial. When q is an integer, equation (2.10) becomes a polynomial of degree $2q - 1$. See (3.1) and (3.4). When q is even the degree reduces to $q - 1$ and we compute the exact value of β_4 (3.3). In general, equation (2.10) is transcendental and most likely cannot be solved exactly. We rewrite this in terms of hypergeometric and associated Legendre functions and also show that $\sqrt{2} \leq \beta_q \leq 2$ and is decreasing (Proposition 3.1). In Theorem 3.2 we show how the corrected trapezoidal rule can give good approximations of the integral of f with $f'' \in L^p([a, b])$ for all $1 \leq p \leq \infty$ even if the exact value of β_q is not known. Part (c) of this theorem shows that the corrected trapezoidal rule with $\alpha = 0, \beta = \infty$ gives a smaller error estimate than (1.2) for all $1 \leq q < \infty$. The coefficient is a simple function of q .

If q is an integer, use the binomial theorem to write (2.10) as

$$\int_1^{\beta_q} (x^2 - 1)^{q-1} dx = \sum_{k=0}^{q-1} \binom{q-1}{k} \frac{(-1)^{q-1+k}}{2k+1} [\beta_q^{2k+1} - 1] = \sum_{k=0}^{q-1} \binom{q-1}{k} \frac{(-1)^k}{2k+1}. \tag{3.1}$$

This gives a polynomial of degree $2q - 1$ for β_q . When q is even this reduces to

$$\sum_{k=0}^{q-1} \binom{q-1}{k} \frac{(-1)^k \beta_q^{2k}}{2k+1} = 0. \tag{3.2}$$

When $p = 4/3$ and $q = 4$ we get the polynomial $\beta_4^6 - (21/5)\beta_4^4 + 7\beta_4^2 - 7 = 0$. The unique solution is [16, 1.11(iii)]

$$\beta_4 = \left\{ \frac{2(7^{1/3})}{(32/3)^{5/3}} \left([5\sqrt{30} + 27]^{1/3} - [5\sqrt{30} - 27]^{1/3} \right) + 7/5 \right\}^{1/2} \doteq 1.589291662. \tag{3.3}$$

This can then be used in equations (2.2) and (2.3).

Repeated use of (2.11) yields the equivalent series form of (2.10) when q is an integer

$$\beta_q \sum_{k=0}^{q-1} (-1)^k \binom{2k}{k} \left(\frac{\beta_q^2 - 1}{4} \right)^k = 1 - (-1)^q. \quad (3.4)$$

When q is even this simplifies to

$$\sum_{k=0}^{q-1} \binom{2k}{k} \left(\frac{1 - \beta_q^2}{4} \right)^k = \sum_{k=0}^{q-1} \frac{(1/2)_k}{k!} (1 - \beta_q^2)^k = 0. \quad (3.5)$$

When $p = 3$ and $q = 3/2$ the integrals in (2.10) can be evaluated in terms of elementary functions but this leads to a transcendental equation for $\beta_{3/2}$. Similarly when q is a half integer.

As can be seen from (3.3) the numbers β_q are not necessarily simple functions of q . For cases other than $p = 1, 2, \infty$ they can be numerically approximated and for this there are many other ways (2.10) can be rewritten. For example, using a linear change of variables and then the identities [16, 15.6.1, 15.9.21] the integral in (2.10) can be written in terms of hypergeometric and associated Legendre functions. The result is

$$\begin{aligned} \int_1^{\beta_q} (x^2 - 1)^{q-1} dx &= 2^{q-1} (\beta_q - 1)^q \int_0^1 [1 - (1 - \beta_q)x/2]^{q-1} x^{q-1} dx \\ &= \frac{2^{q-1} (\beta_q - 1)^q}{q} {}_2F_1(1 - q, q; 1 + q; (1 - \beta_q)/2) \\ &= 2^{q-1} \Gamma(q) (\beta_q^2 - 1)^{q/2} P_{q-1}^{-q}(\beta_q). \end{aligned}$$

Numerical equation solvers can now be applied to any of these representations of $\int_1^{\beta_q} (x^2 - 1)^{q-1} dx$ in order to solve (2.10).

The range of β_q is known.

PROPOSITION 3.1. β_q is a decreasing function of q and $\sqrt{2} \leq \beta_q \leq 2$ for $1 \leq q \leq \infty$.

Proof. A change of variables shows that (2.1) is equivalent to $\int_0^{\beta_q^2 - 1} y^{q-1} (1 + y)^{-1/2} dy = J(q)$, where $J(q) = \int_0^1 y^{q-1} (1 - y)^{-1/2} dy$. Since $(1 + y)^{-1/2} \leq (1 - y)^{-1/2}$ for all $0 \leq y < 1$ we must have $\beta_q^2 - 1 \geq 1$.

Equation (2.1) can also be written as $I(q) + 2 \int_{\sqrt{2}}^{\beta_q} (x^2 - 1)^{q-1} dx = J(q)$ where $I(q) = \int_0^1 y^{q-1} (1 + y)^{-1/2} dy$. The argument above shows that $J'(q) < I'(q) < 0$ for all $1 < q < \infty$. Since $\beta_q \geq \sqrt{2}$ it must be a decreasing function of q . \square

Even without knowing the exact value of β_q we can use the method of Theorem 2.1 to obtain good estimates of the error in corrected trapezoidal rules.

THEOREM 3.2. *Let c be the midpoint of $[a, b]$. Let $f: [a, b] \rightarrow \mathbb{R}$ such that f' is absolutely continuous and $f'' \in L^p([a, b])$ for some $1 \leq p < \infty$. (a) If $1 \leq p < 2$ let $\phi(x) = (x - c)^2 - (b - a)^2/8$. Equation (1.1) gives the quadrature formula*

$$\int_a^b f(x) dx = \frac{(b-a)}{2} [f(a) + f(b)] + \frac{(b-a)^2}{16} [f'(a) - f'(b)] + E(f), \quad (3.6)$$

where the error satisfies $|E(f)| \leq \|f''\|_1 (b-a)^2/16$. (b) If $2 \leq p < \infty$ let $\phi(x) = (x - c)^2 - (b - a)^2/12$. Equation (1.1) gives the quadrature formula

$$\int_a^b f(x) dx = \frac{(b-a)}{2} [f(a) + f(b)] + \frac{(b-a)^2}{12} [f'(a) - f'(b)] + E(f), \quad (3.7)$$

where the error satisfies $|E(f)| \leq \|f''\|_2 (b-a)^{2.5}/(12\sqrt{5})$. (c) If $1 < p < \infty$ let $\phi(x) = (x - c)^2$ and $1/p + 1/q = 1$. Equation (1.1) gives the quadrature formula

$$\int_a^b f(x) dx = \frac{(b-a)}{2} [f(a) + f(b)] + \frac{(b-a)^2}{8} [f'(a) - f'(b)] + E(f), \quad (3.8)$$

where the error satisfies

$$|E(f)| \leq \frac{\|f''\|_p (b-a)^{2+1/q}}{2^{3+1/q} (q+1/2)^{1/q}}. \quad (3.9)$$

Proof. Use the fact that $L^s([a, b]) \subset L^r([a, b])$ whenever $1 \leq r \leq s \leq \infty$. In (a) use the approximation from Corollary 2.2 and in (b) use the approximation from Corollary 2.3. In (c) take $\alpha = 0$, $\beta = \infty$ and then compute

$$\|\phi\|_q^q = 2 \left(\frac{b-a}{2} \right)^{2q+1} \int_0^1 x^{2q} dx = \frac{(b-a)^{2q+1}}{2^{2q+1} (q+1/2)}.$$

The rest follows as in the proof of Theorem 2.1. \square

It is also possible to compute $\|\phi\|_q$ when $\beta = 1$ but this gives the trapezoidal rule (1.2). Note that the coefficient in part (c) is strictly less than the corresponding coefficient in (1.2) for all $1 \leq q < \infty$. In the limit $q \rightarrow \infty$ the coefficient becomes $1/8$ as in (1.2).

4. Lemmas

Let \mathcal{P}_m be the set of monic polynomials of degree $m \in \mathbb{N}$ with real coefficients. Define $F_q: \mathcal{P}_m \rightarrow \mathbb{R}$ by $F_q(\phi) = \|\phi\|_q$ where $1 \leq q \leq \infty$ and the norms are over compact interval $[a, b]$. Since $F_q(\phi)$ is bounded below for $\phi \in \mathcal{P}_m$ it has an infimum over \mathcal{P}_m . It also has a unique minimum at a polynomial that has m roots in $[a, b]$. As well, the error-minimizing polynomial is even or odd about the midpoint of $[a, b]$ as m is even or odd.

LEMMA 4.1. (a) For $m \geq 2$, let $\phi \in \mathcal{P}_m$ with a non-real root. There exists $\psi \in \mathcal{P}_m$ with a real root such that $F_q(\psi) < F_q(\phi)$. (b) Let $\phi \in \mathcal{P}_m$ with a root $t \notin [a, b]$. There exists $\psi \in \mathcal{P}_m$ with a root in $[a, b]$ such that $F_q(\psi) < F_q(\phi)$. (c) If ϕ minimizes F_q then it has m simple zeros in $[a, b]$. (d) If F_q has a minimum in \mathcal{P}_m it is unique. (e) F_q attains its minimum over \mathcal{P}_m . (f) If $\phi \in \mathcal{P}_m$ is neither even nor odd about $c := (a+b)/2$ then there is a polynomial $\psi \in \mathcal{P}_m$ that is either even or odd about c such that $F_q(\psi) < F_q(\phi)$. (g) The minimum of F_q occurs at a polynomial $\phi \in \mathcal{P}_m$ with m simple zeros in $[a, b]$. If m is even about c then so is ϕ . If m is odd about c then so is ϕ . This minimizing polynomial is unique.

Theorem 2.1 and its corollaries used only \mathcal{P}_2 but the lemmas give results for \mathcal{P}_m for all m . These will be useful for considering integration schemes generated by polynomials of degree m , which we do not include here.

The results of Lemma 4.1 are well known and go back to Chebyshev and Fejér. To keep the paper self contained we have provided elementary proofs. For a full exposition and references to the original literature see, for example, [5], [7] and [15]. Three cases of the minimizing problem of Lemma 4.1 appear in the literature. When $q = \infty$ the minimizing polynomial in \mathcal{P}_2 is the Chebyshev polynomial of the first kind $\phi(x) = x^2 - 1/2 = T_2(x)/2$. When $q = 2$ it is given as a Legendre polynomial $\phi(x) = x^2 - 1/3 = (2/3)P_2(x)$. When $q = 1$ it is the Chebyshev polynomial of the second kind $\phi(x) = x^2 - 1/4 = U_2(x)/4$. These are for the interval $[-1, 1]$. A linear change of variables is used for other intervals. These are all types of Gegenbauer polynomials, which are orthogonal on $[-1, 1]$ with respect to a certain weight function. Gillis and Lewis [11] give an argument to show that the minimizing polynomials are most likely not orthogonal polynomials for other values of q .

Proof. (a) Write $\phi(x) = [(x-r)^2 + s^2]\omega(x)$ for some $r, s \in \mathbb{R}$, $s \neq 0$, and $\omega \in \mathcal{P}_{m-2}$. Let $\psi(x) = (x-r)^2\omega(x)$. For all $x \in \mathbb{R}$ such that $\omega(x) \neq 0$ we have $|\psi(x)| < |\phi(x)|$. Hence, $\|\psi\|_q < \|\phi\|_q$.

(b) If $m = 1$ let $\phi(x) = x - t$. Direct calculation shows the unique minimum of $\|\phi\|_q$ occurs at $t = c$. If $m \geq 2$, by (a) we can assume all the roots of ϕ are real and write $\phi(x) = (x-t)\omega(x)$ for some $t \notin [a, b]$, and $\omega \in \mathcal{P}_{m-1}$. Suppose $t < a$. Let $\psi(x) = (x-a)\omega(x)$. For all $x \in [a, b]$ such that $\omega(x) \neq 0$ we have $|\psi(x)| < |\phi(x)|$. Hence, $\|\psi\|_q < \|\phi\|_q$. Similarly if $t > b$.

(c) Consider $\psi(x) = (x-t)^2$ with $t \in (a, b)$ and $\psi_\varepsilon(x) = (x-t+\varepsilon)(x-t-\varepsilon) = \psi(x) - \varepsilon^2$. For all x we have $|\psi_\varepsilon(x)| \leq |\psi(x)| + \varepsilon^2$ and for $x \notin (t-\varepsilon, t+\varepsilon)$ we have $|\psi_\varepsilon(x)| < |\psi(x)|$. This shows that $\|\psi_\varepsilon\|_\infty < \|\psi\|_\infty$ if $\varepsilon > 0$ is small enough. Factoring now shows the zeros of any minimizing polynomial are simple. Similarly for $t = a$ or b .

For $q = 1$,

$$\begin{aligned} \|\psi_\varepsilon\|_1 &= \int_{x \in (t-\varepsilon, t+\varepsilon)} [\varepsilon^2 - \psi(x)] dx + \int_{x \notin (t-\varepsilon, t+\varepsilon)} [\psi(x) - \varepsilon^2] dx \\ &\leq \|\psi\|_1 + 4\varepsilon^3 - \varepsilon^2(b-a) \\ &< \|\psi\|_1 \quad \text{for small enough } \varepsilon > 0. \end{aligned}$$

And, if $g \in L^\infty([a, b])$ such that $|g| > 0$ almost everywhere then $\|\psi_\varepsilon g\|_1 < \|\psi g\|_1$ for small enough $\varepsilon > 0$. A similar construction is used when t equals a or b . Factoring ψ shows the zeros of any minimizing polynomial must be simple.

For $1 < q < \infty$ use the same construction, with Taylor’s theorem in (4.1), to get

$$\begin{aligned} \|\psi_\varepsilon\|_q^q &= \int_{x \in (t-\varepsilon, t+\varepsilon)} [\varepsilon^2 - \psi(x)]^q dx + \int_{x \notin (t-\varepsilon, t+\varepsilon)} [\psi(x) - \varepsilon^2]^q dx \\ &\leq \int_{x \in (t-\varepsilon, t+\varepsilon)} \varepsilon^{2q} dx + \int_{x \notin (t-\varepsilon, t+\varepsilon)} \psi^q(x) - q\varepsilon^2 [\psi(x) - \varepsilon^2]^{q-1} dx \quad (4.1) \\ &< 2\varepsilon^{2q+1} + \|\psi\|_q^q - q\varepsilon^2 \int_{x \notin (t-2\varepsilon, t+2\varepsilon)} (3\varepsilon^2)^{q-1} dx \\ &= 2\varepsilon^{2q+1} + \|\psi\|_q^q - 3^{q-1} q \varepsilon^{2q} (b-a-4\varepsilon) \\ &< \|\psi\|_q^q \quad \text{for small enough } \varepsilon > 0. \end{aligned}$$

As with the $q = 1$ case above, it now follows that zeros of minimizing polynomials must be simple.

(d) Suppose the minimum of F_q occurs at both $\phi, \omega \in \mathcal{P}_m$. Let $\psi = (\phi + \omega)/2$. Then $\psi \in \mathcal{P}_m$ so $\|\phi\|_q \leq \|\psi\|_q \leq (\|\phi\|_q + \|\omega\|_q)/2 = \|\phi\|_q$. The Minkowski inequality must then reduce to equality. For $1 < q < \infty$ this means $\phi = d\omega$ for some $d > 0$ [13, p. 47]. Since $\phi, \omega \in \mathcal{P}_m$ we must have $d = 1$. If $q = 1$ then there is equality in the Minkowski inequality if and only if $\phi\omega \geq 0$. If there is equality, then ϕ and ψ must share roots of odd multiplicity. But by (c), ϕ and ψ have m simple zeros in $[a, b]$. Hence, $\phi = \psi$. For $q = \infty$, Lemma 4.2 shows there are $a < x_1 < \dots < x_{m-1} < b$, $a < y_1 < \dots < y_{m-1} < b$ and $a < z_1 < \dots < z_{m-1} < b$ such that $|\phi(x_i)| = |\omega(y_i)| = |\psi(z_i)| = \|\phi\|_\infty$, $\phi'(x_i) = \omega'(y_i) = \psi'(z_i) = 0$ for each $1 \leq i \leq m-1$. Let $M_\phi = \{x_i\}_{i=1}^{m-1}$, $M_\omega = \{y_i\}_{i=1}^{m-1}$, $M_\psi = \{z_i\}_{i=1}^{m-1}$. Let $z \in M_\psi$ then $\|\phi\|_\infty = |\psi(z)| = |\phi(z) + \omega(z)|/2 < \|\phi\|_\infty$ unless $z \in M_\phi \cap M_\omega$. Hence, $M_\phi = M_\omega$. Therefore, $\phi'(x_i) = \psi'(x_i)$ for each $1 \leq i \leq m-1$. And then $\phi = \omega$.

(e) By parts (a) and (b) we need only consider $\phi \in \mathcal{P}_m$ with m real roots in $[a, b]$. Let $t_i \in [a, b]$ for $1 \leq i \leq m$ and define $\phi \in \mathcal{P}_m$ by $\phi(x) = \prod_{i=1}^m (x - t_i)$.

Suppose $1 \leq q < \infty$. Define $G_q(t) = \int_a^b \prod_{i=1}^m |x - t_i|^q dx$. Then $G_q : [a, b]^m \rightarrow \mathbb{R}$ attains its minimum over $[a, b]^m$ if and only if F_q attains its minimum over \mathcal{P}_m . The set $[a, b]^m$ is compact in \mathbb{R}^m . And, G_q is continuous. For, suppose $t \in [a, b]^m$ and $s^{(k)} \in [a, b]^m$ for each $k \in \mathbb{N}$ such that $s^{(k)} \rightarrow t$ in the Euclidean norm. We have

$$\int_a^b \prod_{i=1}^m |x - s_i^{(k)}|^q dx \leq \int_a^b \prod_{i=1}^m (b-a)^q dx = (b-a)^{mq+1}.$$

By dominated convergence (for example, [1, Theorem 7.2]), $\lim_{k \rightarrow \infty} G_q(s^{(k)}) = G_q(t)$ and G_q is continuous. Therefore, G_q attains its minimum over $[a, b]^m$.

The case $q = \infty$ is similar, using $F_\infty(\phi) = \max_{x \in [a, b]} \prod_{i=1}^m |x - t_i|$.

(f) Without loss of generality, $b = -a$. Suppose $\psi \in \mathcal{P}_m$ is the unique minimizer of F_q . Let $\omega(x) = \psi(-x)$ if m is even and $\omega(x) = -\psi(-x)$ if m is odd. Then $\omega \in \mathcal{P}_m$ and $\|\omega\|_q = \|\psi\|_q$. Let $\zeta = (\psi + \omega)/2$. Then $\zeta \in \mathcal{P}_m$ and is even if m is

even, odd if m is odd. Also, $\|\zeta\|_q \leq (\|\psi\|_q + \|\omega\|_q)/2 = \|\psi\|_q$. Hence, $\zeta = \psi = \omega$. But then ψ is even or odd as m is even or odd. If $\phi \in \mathcal{P}_m$ is neither even nor odd then $F_q(\psi) < F_q(\phi)$. \square

LEMMA 4.2. *Suppose $\phi \in \mathcal{P}_m$ is a minimum of F_∞ . Then $\phi(x) = \prod_{i=1}^m (x - t_i)$ for $a < t_1 < t_2 < \dots < t_m < b$. For each $1 \leq i \leq m - 1$ there is $\xi_i \in (t_i, t_{i+1})$ such that $|\phi(\xi_i)| = \|\phi\|_\infty$.*

Proof. This follows from the $q = \infty$ case of Lemma 4.1(c). \square

5. f'' Henstock–Kurzweil integrable

Let $HK([a, b])$ be the set of functions integrable in the Henstock–Kurzweil sense on $[a, b]$. See, for example, [12]. Note that $L^s([a, b]) \subsetneq L^r([a, b]) \subsetneq HK([a, b])$ for all $1 \leq r < s \leq \infty$. An example of a function $f \in HK([0, 1])$ that is not in any $L^p([0, 1])$ space is $f = F'$ where $F(x) = x^2 \sin(x^{-3})$ for $x \in (0, 1]$ and $F(x) = 0$. In this section we use the method of Theorem 2.1 to choose a monic quadratic ϕ to minimize the error in the resulting corrected trapezoidal rule when $f'' \in HK([a, b])$. We also consider the case when f' is merely continuous and then f'' exists as a distribution. For all of these cases, it turns out that amongst corrected trapezoidal rules (1.1), the trapezoidal rule itself minimizes the error.

If $f \in HK([a, b])$ then the Alexiewicz norm of f is $\|f\| = \sup_{x \in [a, b]} |\int_a^x f(t) dt|$. If $g : [a, b] \rightarrow \mathbb{R}$ is of bounded variation then $fg \in HK([a, b])$. Integration by parts shows that $|\int_a^b f(x)g(x) dx| \leq |\int_a^b f|g(b)| + \|f\|Vg$, where Vg is the variation of g . This is a version of an inequality known in the literature as the Darst–Pollard–Beesack inequality. See [6], [2]. However, it appears earlier in [18]. It is proved for a more symmetric version of the Alexiewicz norm for Henstock–Kurzweil integrals in [19, Lemma 24].

Under the Alexiewicz norm, $HK([a, b])$ is a normed linear space but is not complete. We will discuss integration in the completion later in this section.

THEOREM 5.1. *Let c be the midpoint of $[a, b]$. Let $f : [a, b] \rightarrow \mathbb{R}$ such that $f' \in C([a, b])$ and $f'' \in HK([a, b])$. Amongst all monic quadratic polynomials used to generate (1.1), taking $\phi(x) = (x - c)^2 - (b - a)^2/4 = (x - a)(x - b)$ minimizes the error $|E(f)|$. This gives the quadrature formula*

$$\int_a^b f(x) dx = \frac{b-a}{2} [f(a) + f(b)] + E(f), \quad (5.1)$$

where

$$|E(f)| \leq \|f''\| (b-a)^2/4. \quad (5.2)$$

For a uniform partition given by $x_i = a + (b-a)i/n$, $0 \leq i \leq n$, the composite formula is the trapezoidal rule

$$\int_a^b f(x) dx = \frac{b-a}{2n} \left[f(a) + 2 \sum_{i=1}^{n-1} f(x_i) + f(b) \right] + E(f), \quad (5.3)$$

where

$$|E(f)| \leq \frac{\|f''\|(b-a)^2}{4n}.$$

The coefficient of $\|f''\|$ in the error bounds is the best possible.

Proof. From (1.1) we have $|E(f)| \leq (\int_a^b f''(x) dx |\phi(b)| + \|f''\| V\phi)/2$. Write $\phi(x) = (x-r)^2 + s$. Then $V\phi = 2 \int_a^b |x-r| dx$. This is minimized when $r = c$. Note that $\phi(b) = 0$ if and only if $s = -(b-a)^2/4$. The unique error-minimizing polynomial is then $\phi(x) = (x-c)^2 - (b-a)^2/4 = (x-a)(x-b)$, for which $V\phi = (b-a)^2/2$. Hence, $|E(f)| \leq \|f''\|(b-a)^2/4$. To show this estimate cannot be improved, let (ψ_n) be a delta sequence as in the proof of Corollary 2.2. Define $f_n''(x) = \psi_n(x-a) - 2\psi_n(x-c) + \psi_n(b-x)$. Then $\int_a^b f_n''(x) dx = 0$ and $\|f_n''\| = 1$. Integrate to get $f_n(x) = \int_a^x (x-t)f_n''(t) dt$, modulo a linear function. Since ϕ is continuous, $\lim_{n \rightarrow \infty} |\int_a^b f_n''(x)\phi(x) dx| = |\phi(a) - 2\phi(c) + \phi(b)| = (b-a)^2/2$. \square

In the terminology of Theorem (2.1) the minimizing polynomial has $\beta = 1$ and $\alpha = (b-a)/2$ and is the same as the one that generated the trapezoidal rule in (1.2). Notice that the variation is additive over disjoint intervals so the error in the composite formula is order $1/n$, compared with error of order $1/n^2$ in Corollary 2.5 when $f'' \in L^p[a, b]$.

An equivalent norm is $\|f\|^* = \sup_I |\int_I f(x) dx|$ where the supremum is taken over all intervals $I \subset [a, b]$. It is easy to see that $\|f\| \leq \|f\|^* \leq 2\|f\|$ for all $f \in HK([a, b])$. In terms of this norm, (5.2) implies $|E(f)| \leq \|f''\|^*(b-a)^2/4$. This inequality appears as Theorem 21 in [10]. We improve this inequality by a factor of $1/2$ and show our result is sharp.

COROLLARY 5.2. *With the assumptions of Theorem 5.1 we have $|E(f)| \leq (b-a)^2 \|f''\|^*/8$. The constant $1/8$ is the best possible.*

Proof. Use the second mean value theorem for integrals [3]. If ϕ is monotonic on $[a, b]$ then there is $\xi \in [a, b]$ such that

$$E(f) = \frac{1}{2} \int_a^b f''(x)\phi(x) dx = \frac{\phi(a)}{2} \int_a^\xi f''(x) dx + \frac{\phi(b)}{2} \int_\xi^b f''(x) dx.$$

Then $|E(f)| \leq (|\phi(a)| + |\phi(b)|) \|f''\|^*/2$. This is minimized by taking $\phi(x) = (x-a)^2$ or $\phi(x) = (x-b)^2$, for which $|E(f)| \leq (b-a)^2 \|f''\|^*/2$. If ϕ has a minimum at $r \in (a, b)$ then there are $\xi_1 \in [a, r]$ and $\xi_2 \in [r, b]$ such that

$$E(f) = \frac{\phi(a)}{2} \int_a^{\xi_1} f''(x) dx + \frac{\phi(r)}{2} \int_{\xi_1}^r f''(x) dx + \frac{\phi(r)}{2} \int_r^{\xi_2} f''(x) dx + \frac{\phi(b)}{2} \int_{\xi_2}^b f''(x) dx.$$

It follows that $|E(f)| \leq (|\phi(a)| + |\phi(r)| + |\phi(b)|) \|f''\|^*/2$. Choosing $\phi(x) = (x-a)(x-b)$ minimizes the coefficient of $\|f''\|^*$ and we get $|E(f)| \leq (b-a)^2 \|f''\|^*/8$. To prove this estimate is sharp, let (ψ_n) be a delta sequence as in the proof of Corollary 2.2.

Define $f_n''(x) = \psi_n(x - c)$. Then $\|f_n''\|^* = 1$ and $|E(\psi_n)| \rightarrow (c - a)(b - c)/2 = (b - a)^2/8$. \square

The completion of $HK([a, b])$ in the Alexiewicz norm is the Banach space $\mathcal{A}_c([a, b])$. Each element of $\mathcal{A}_c([a, b])$ is the distributional derivative of a function in $\mathcal{B}_c([a, b]) = \{F \in C([a, b]) \mid F(a) = 0\}$. Note that $\mathcal{B}_c([a, b])$ is a Banach space under usual pointwise operations and the uniform norm. If $f \in \mathcal{A}_c([a, b])$ then there is a unique primitive $F \in \mathcal{B}_c([a, b])$ such that $F' = f$. The distributional derivative is $\langle F', \phi \rangle = -\langle F, \phi' \rangle = -\int_a^b F(x)\phi'(x) dx$ where $\phi \in C_c^\infty(\mathbb{R})$. The Alexiewicz norm of f is $\|f\| = \sup_{x \in [a, b]} |\int_a^x f| = \|F\|_\infty$. This makes $\mathcal{A}_c([a, b])$ into a Banach space isometrically isomorphic to $\mathcal{B}_c([a, b])$. The continuous primitive integral of $f \in \mathcal{A}_c([a, b])$ is then $\int_a^b f = F(b) - F(a)$. If g is of bounded variation then the integration by parts formula is given in terms of a Riemann–Stieltjes integral as $\int_a^b fg = F(b)g(b) - \int_a^b F(x) dg(x)$. Note that $\mathcal{A}_c([a, b])$ contains $HK([a, b])$ and hence $L^p([a, b])$ for each $1 \leq p \leq \infty$. If F is a continuous function such that its pointwise derivative $F'(x) = 0$ almost everywhere then the Lebesgue integral of $F'(x)$ exists and is 0 but the continuous primitive integral is $\int_a^b F' = F(b) - F(a)$. If F is continuous such that the pointwise derivative exists nowhere then the Lebesgue integral of $F'(x)$ does not exist but $F' \in \mathcal{A}_c([a, b])$ and $\int_a^b F' = F(b) - F(a)$. See [20] for details. Note that if $F \in C([a, b])$ then $F' \in \mathcal{A}_c([a, b])$ and $\int_a^b F' = F(b) - F(a)$. An advantage of the continuous primitive integral is that the space of primitives is simple. It is the continuous functions while for the Henstock–Kurzweil integral it is a complicated space called ACG^* . See [3] for the definition.

COROLLARY 5.3. *Let $f \in C^1([a, b])$. Then $f'' \in \mathcal{A}_c([a, b])$ and the formulas in Theorem 5.1 hold.*

In a sense this now reduces to estimates on f' since the Alexiewicz norm of f'' is the uniform norm of f' . The formulas in Theorem 5.1 also hold when f' is a regulated function. This is a function that has a left limit and a right limit at each point. See [21] for details.

6. Exact for cubics

In this section we show (1.1) is exact for all ϕ when f is a linear function. We also show (1.1) is exact for all cubic polynomials f whenever $\phi(x) = (x - c)^2 - (b - a)^2/12$.

THEOREM 6.1. *Let $f: [a, b] \rightarrow \mathbb{R}$ and let c be the midpoint of $[a, b]$. Let ϕ be a monic quadratic. Write*

$$\int_a^b f(x) dx = \frac{1}{2} [-f(a)\phi'(a) + f(b)\phi'(b) + f'(a)\phi(a) - f'(b)\phi(b)] + E(f). \quad (6.1)$$

(a) *If f is a linear function then $E(f) = 0$ for all such ϕ . (b) $E(f) = 0$ for all cubic polynomials f if and only if $\phi(x) = (x - c)^2 - (b - a)^2/12$.*

Proof. The proof of (a) is straightforward using $E(f) = (1/2) \int_a^b f''(x)\phi(x) dx$. By (a) we need only consider $f(x) = Ax^3 + Bx^2$. Write $\phi(x) = x^2 + Cx + D$. The equation $\int_a^b (6Ax + 2B)(x^2 + Cx + D) dx = 0$ gives the linear system

$$2(a^2 + ab + b^2)C + 3(a + b)D = -\frac{3}{2}(a + b)(a^2 + b^2) \quad (6.2)$$

$$(a + b)C + 2D = -\frac{2}{3}(a^2 + ab + b^2). \quad (6.3)$$

The solution is $C = -(a + b)$, $D = (a^2 + 4ab + b^2)/6$, and this gives $\phi(x) = (x - c)^2 - (b - a)^2/12$. \square

Note that this is the same ϕ as in Corollary 2.3. Also, $E(f) = 0$ for all quadratic polynomials f if and only if (6.3) holds.

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