ON SPECTRAL ACCURACY OF QUADRATURE FORMULAE BASED ON PIECEWISE POLYNOMIAL INTERPOLATION

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Abstract. It is well-known that the trapezoidal rule, while being only second-order accurate in general, improves to spectral accuracy if applied to the integration of a smooth periodic function over an entire period on a uniform grid. More precisely, for the function that has a square integrable derivative of order r the convergence rate is $o\left(N^{-(r-1/2)}\right)$, where N is a number of grid nodes. Accordingly, for a C^∞-function the trapezoidal quadrature converges with the rate faster than any polynomial. In this paper, we prove that the same property holds for all quadrature formulae obtained by integrating fixed degree piecewise polynomial interpolations of a smooth integrand, such as the midpoint rule, Simpson's rule, etc.

Key words. Numerical quadrature, piecewise polynomial, convergence rate, trapezoidal rule, midpoint rule, Simpson's rule, spectral accuracy.

Let $f = f(x)$ be a function defined in the interval $a \le x \le b$, $|b-a| = L$. To approximate the value of its integral $\displaystyle\int_a^b f(x)\,dx$, let us introduce a partition of the interval $[a,b]$ into N equal subintervals of size $h = L/N$. The partition is rendered by the nodes of the grid: $x_j = a + jh$, $j = 0,1,\dots,N$, so that $x_0 = a$ and $x_N = b$. On each subinterval $[x_j, x_{j+1}]$, $j = 0,1,\dots,N-1$, we approximate the function f by the interpolating polynomial of degree 1:

$$f(x) \approx Q_1(x,f,x_j,x_{j+1}) = f_j\frac{x_{j+1}-x}{h} + f_{j+1}\frac{x-x_j}{h}, \tag{1}$$

where $f_j = f(x_j)$, $j = 0,1,\dots,N$. Then, by replacing $f(x)$ with the corresponding linear interpolant (1) on each subinterval, one obtains *the trapezoidal quadrature rule*:

$$\begin{aligned}\int_a^b f(x)\,dx &\approx \sum_{j=0}^{N-1}\int_{x_j}^{x_{j+1}} Q_1(x,f,x_j,x_{j+1})\,dx = \sum_{j=0}^{N-1}\left(f_j\frac{h}{2} + f_{j+1}\frac{h}{2}\right)\\ &= h\left(\frac{f_0}{2} + f_1 + f_2 + \ldots + f_{N-1} + \frac{f_N}{2}\right).\end{aligned} \tag{2}$$

It is well-known that if the second derivative $f''(x)$ is bounded on $[a,b]$, then the interpolation error in formula (1) is:

$$f(x) - Q_1(x,f,x_j,x_{j+1}) = \frac{f''(\xi)}{2!}(x-x_j)(x-x_{j+1}), \tag{3}$$

where $\xi = \xi(x) \in [x_j, x_{j+1}]$. Therefore,

$$|f(x) - Q_1(x,f,x_j,x_{j+1})| \le \frac{1}{8}\max_{x_j\le x\le x_{j+1}}|f''(x)|h^2 \le \frac{1}{8}\max_{a\le x\le b}|f''(x)|h^2.$$

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Consequently, the error of the trapezoidal rule (2) can be estimated as:

$$\left| \int_a^b f(x)\,dx - h\sum_{j=0}^{N-1}\left(\frac{f_j}{2}+\frac{f_{j+1}}{2}\right)\right| \le \sum_{j=0}^{N-1}\left| \int_{x_j}^{x_{j+1}} (f(x)-Q_1(x,f,x_j,x_{j+1}))\,dx\right| \le$$
$$\sum_{j=0}^{N-1}\int_{x_j}^{x_{j+1}} |f(x)-Q_1(x,f,x_j,x_{j+1})|\,dx \le \frac{N}{8}\max_{a\le x\le b}|f''(x)|h^3 = \frac{L}{8}\max_{a\le x\le b}|f''(x)|h^2.$$

In other words, when $h \to 0$, the error of the trapezoidal rule decays at least as fast as $\mathcal{O}(h^2)$. It is important to emphasize that *in general this estimate cannot be improved.* Namely, even if the function $f(x)$ has bounded derivatives of order higher than two on $[a, b]$, the convergence of the trapezoidal rule will still remain quadratic. This immediately follows from the fact that even for smoother functions the interpolation error is given by the same formula (3).

However, there is one particular case when the trapezoidal rule provides a much better accuracy of approximation. This is the case of a smooth and L-periodic function f, for which the rate of convergence of the trapezoidal quadrature will automatically adjust to the degree of regularity of f. In the literature, this result is commonly referred to as standard; a proof, for instance, can be found in [2, Section 2.9] or in [3, Section 4.1.2]. Moreover, this result has far-reaching implications in scientific computation; it facilitates construction of efficient numerical methods, for example, in the scattering theory, see [1]. Since one can actually come across several slightly different versions of this result, we formulate it as a theorem and provide a proof that follows [3] and is based on a simpler argument than the one used in [2].

Theorem 1. *Let $f = f(x)$ be an L-periodic function and assume that its derivative of order r is square integrable: $f^{(r)} \in L^2$. Then the error of the trapezoidal quadrature rule (2) can be estimated as:*

$$\left| \int_a^{a+L} f(x)\,dx - h\sum_{j=0}^{N-1}\left(\frac{f_j}{2}+\frac{f_{j+1}}{2}\right)\right| \le L\cdot\frac{\zeta_N}{N^{r-1/2}}, \tag{4}$$

where $\zeta_N \to 0$ as $N \to \infty$.

Proof. We first note that since the function f is integrated over a full period, we may assume without loss of generality that $a = 0$. We then represent f as the sum of its Fourier series:

$$f(x) = S_{N-1}(x) + R_{N-1}(x), \tag{5}$$

where

$$S_{N-1}(x) = \frac{a_0}{2} + \sum_{n=1}^{N-1} a_n \cos\frac{2\pi nx}{L} + \sum_{n=1}^{N-1} b_n \sin\frac{2\pi nx}{L} \tag{6}$$

is the partial sum of order $N-1$ and

$$R_{N-1}(x) = \sum_{n=N}^{\infty} a_n \cos\frac{2\pi nx}{L} + \sum_{n=N}^{\infty} b_n \sin\frac{2\pi nx}{L} \tag{7}$$

is the corresponding remainder. The coefficients a_n and b_n of the Fourier series of f are given by the formulae:

$$a_n = \frac{2}{L}\int_0^L f(x)\cos\frac{2\pi nx}{L}\,dx, \qquad b_n = \frac{2}{L}\int_0^L f(x)\sin\frac{2\pi nx}{L}\,dx. \tag{8}$$

Notice that according to formulae (6) and (8), the following equality holds:

$$\frac{L}{2}a_0 = \int_0^L S_{N-1}(x)\,dx = \int_0^L f(x)\,dx. \tag{9}$$

We now integrate equality (5) over $[0, L]$:

$$\int_0^L f(x)\,dx = \int_0^L S_{N-1}(x)\,dx + \int_0^L R_{N-1}(x)\,dx. \tag{10}$$

and apply the trapezoidal quadrature rule to the right-hand side (RHS) of (10). For the first integral there, this can be done via the term-by-term integration of (6). We start with the constant component ($n = 0$), for which, taking into account (9), we immediately get:

$$h\sum_{j=0}^{N-1}\left(\frac{a_0/2}{2} + \frac{a_0/2}{2}\right) = \frac{L}{2}a_0 = \int_0^L S_{N-1}(x)\,dx = \int_0^L f(x)\,dx.$$

For all other terms ($n = 1, 2, \dots, N-1$) we exploit periodicity with the period L, use the definition of the grid size $h = L/N$, and obtain:

$$h\sum_{j=0}^{N-1}\left(\frac{a_n}{2}\cos\frac{2\pi njh}{L} + \frac{a_n}{2}\cos\frac{2\pi n(j+1)h}{L}\right) = a_n h\sum_{j=0}^{N-1}\cos\frac{2\pi njh}{L}$$
$$= \frac{a_n h}{2}\sum_{j=0}^{N-1}\left(e^{i\frac{2\pi njh}{L}} + e^{-i\frac{2\pi njh}{L}}\right) = \frac{a_n h}{2}\left(\frac{1 - e^{i\frac{2\pi nNh}{L}}}{1 - e^{i\frac{2\pi nh}{L}}} + \frac{1 - e^{-i\frac{2\pi nNh}{L}}}{1 - e^{-i\frac{2\pi nh}{L}}}\right) = 0.$$

Similarly, one can show that

$$h\sum_{j=0}^{N-1}\left(\frac{b_n}{2}\sin\frac{2\pi njh}{L} + \frac{b_n}{2}\sin\frac{2\pi n(j+1)h}{L}\right) = 0.$$

Altogether we conclude that the trapezoidal rule is exact for the partial sum S_{N-1} given by formula (6), namely:

$$h\sum_{j=0}^{N-1}\left(\frac{S_{N-1}(x_j)}{2} + \frac{S_{N-1}(x_{j+1})}{2}\right) = \int_0^L S_{N-1}(x)\,dx = \frac{L}{2}a_0. \tag{11}$$

We also note that choosing the partial sum of order $N-1$, while the number of grid cells being N, is not accidental. From the previous derivation is is easy to see that equality (11) would no longer hold already if we were to take $S_N(x)$ instead of $S_{N-1}(x)$ there.

Next, we need to apply the trapezoidal rule to the remainder of the series R_{N-1} given by formula (7). First we recall that the magnitude of the remainder or, equivalently, the rate of convergence of the Fourier series, is determined by the smoothness of the function f. More precisely, one can show that for a function f such that $f^{(r)} \in L^2$ the following estimate holds:

$$\sup_{0\le x\le L}|R_{N-1}(x)| \le \frac{\zeta_N}{N^{r-1/2}}, \tag{12}$$

where $\zeta_N \to 0$ as $N \to \infty$. Therefore,

$$\left| h \sum_{j=0}^{N-1} \left(\frac{R_{N-1}(x_j)}{2} + \frac{R_{N-1}(x_{j+1})}{2} \right) \right| \le Nh \sup_{0 \le x \le L} |R_{N-1}(x)| = L \cdot \frac{\zeta_N}{N^{r-1/2}}. \tag{13}$$

Finally, we combine formulae (11) and (13) to conclude with:

$$\begin{aligned} &\left| \int_0^L f(x)\,dx - h \sum_{j=0}^{N-1} \left(\frac{f_j}{2} + \frac{f_{j+1}}{2} \right) \right| \\ &= \left| \frac{L}{2} a_0 - h \sum_{j=0}^{N-1} \left(\frac{S_{N-1}(x_j)}{2} + \frac{S_{N-1}(x_{j+1})}{2} + \frac{R_{N-1}(x_j)}{2} + \frac{R_{N-1}(x_{j+1})}{2} \right) \right| \\ &= \left| h \sum_{j=0}^{N-1} \left(\frac{R_{N-1}(x_j)}{2} + \frac{R_{N-1}(x_{j+1})}{2} \right) \right| \le L \cdot \frac{\zeta_N}{N^{r-1/2}}, \end{aligned}$$

which completes the proof of the theorem. □

Remark. If $f \in C^\infty$, then Theorem 1 implies spectral convergence of the trapezoidal quadrature rule. In other words, the rate of decay of the error will be faster than any polynomial, that is, faster than $\mathcal{O}(N^{-r})$ for any $r > 0$.

Let us now consider the entire family of approximate quadratures obtained, like the trapezoidal rule, by integrating piecewise polynomial interpolants of a given fixed degree. Let $N = PM$, where P and M are positive integers. Then, we partition the original grid of N cells into P clusters of M cells each, and within every cluster approximate the function f as follows:

$$\begin{aligned} &f(x) \approx Q_d(x, f, x_{pM}, x_{pM+1}, \dots, x_{(p+1)M}), \\ &x \in [x_{pM}, x_{(p+1)M}], \quad p = 0, 1, \dots, P-1, \end{aligned} \tag{14}$$

where $Q_d(x, f, x_{pM}, x_{pM+1}, \dots, x_{(p+1)M})$ is a unique algebraic interpolating polynomial of degree $d \le M$ that coincides with the function $f(x)$ at the nodes x_j, $j = pM, pM+1, \dots, (p+1)M$.

By integrating the interpolating polynomials (14) over the corresponding cell clusters we arrive at the following approximate quadrature formula:

$$\begin{aligned} \int_a^b f(x)\,dx &\approx \sum_{p=0}^{P-1} \int_{x_{pM}}^{x_{(p+1)M}} Q_d(x, f, x_{pM}, x_{pM+1}, \dots, x_{(p+1)M})\,dx \\ &= h \sum_{p=0}^{P-1} \left(c_0 f_{pM} + c_1 f_{pM+1} + \ldots + c_M f_{(p+1)M} \right), \end{aligned} \tag{15}$$

where the coefficients $c_0, c_1, \dots, c_M$, are uniquely defined for a given M. For example, for the previously analyzed trapezoidal rule (2) we have $P = N$, $M = 1$, $c_0 = 1/2$, and $c_1 = 1/2$. For the well-known Simpson's rule we have $P = N/2$, $M = 2$, $c_0 = 1/3$, $c_1 = 4/3$, and $c_2 = 1/3$. An obvious important property of the quadrature coefficients follows from applying formula (15) to $f(x) \equiv \text{const}$:

$$c_0 + c_1 + \ldots + c_M = M. \tag{16}$$

Typically, the accuracy of the quadrature formulae (15) is $\mathcal{O}(h^{M+1})$, provided that the function f has a bounded derivative of order $M+1$. Sometimes, symmetries may lead to a somewhat better accuracy. For example, the accuracy of Simpson's rule is, in fact, $\mathcal{O}(h^4)$ rather than $\mathcal{O}(h^3)$, provided that $f^{(4)}$ is bounded. *However, for smooth periodic functions f all quadrature formulae of type (15) attain spectral accuracy when applied on a full period.* This is the central result of our note, which we present in the following theorem.

THEOREM 2. *Let $f = f(x)$ be an L-periodic function and assume that its derivative of order r is square integrable: $f^{(r)} \in L^2$. Then the approximation error of any quadrature formula of type (15) can be estimated as:*

$$\left| \int\limits_a^{a+L} f(x)\,dx - h\sum_{p=0}^{P-1}\left(c_0 f_{pM} + \ldots + c_M f_{(p+1)M}\right)\right| \le L\cdot\frac{\zeta_N}{N^{r-1/2}}, \tag{17}$$

where $\zeta_N \to 0$ as $N \to \infty$.

Proof. The proof of the theorem is based on a reduction of the quadrature formula (15) to a linear combination of the trapezoidal-type quadratures, for which estimate (17) reduces to estimate (4) that was proved in Theorem 1. Namely, we can rewrite the quadrature formula (15) as:

$$\begin{aligned} & h\sum_{p=0}^{P-1}\left(c_0 f_{pM} + c_1 f_{pM+1} + \ldots + c_M f_{(p+1)M}\right) \\ &= h\big(c_0 f_0 + (c_0+c_M) f_M + (c_0+c_M) f_{2M} + \ldots + (c_0+c_M) f_{(P-1)M} + c_M f_{PM}\big) \\ &+ h\sum_{m=1}^{M-1} c_m \left(f_m + f_{m+M} + f_{m+2M} + \ldots + f_{m+(P-1)M}\right). \end{aligned}$$

Next, we introduce the ghost nodes of the grid: $\{x_j\}$ for $j = N+1,\ldots,N+M-1$ (or equivalently, $j = PM+1,\ldots,PM+M-1$), and use the L-periodicity of $f(x)$ to recast the previous equality as follows:

$$\begin{aligned} & h\sum_{p=0}^{P-1}\left(c_0 f_{pM} + c_1 f_{pM+1} + \ldots + c_M f_{(p+1)M}\right) \\ &= h\left(\frac{c_0+c_M}{2} f_0 + (c_0+c_M) f_M + \ldots + (c_0+c_M) f_{(P-1)M} + \frac{c_0+c_M}{2} f_{PM}\right) \\ &+ h\sum_{m=1}^{M-1} c_m \left(\frac{f_m}{2} + f_{m+M} + f_{m+2M} + \ldots + f_{m+(P-1)M} + \frac{f_{m+PM}}{2}\right). \end{aligned}$$

We therefore have:

$$\begin{aligned} & \sum_{p=0}^{P-1}\left(c_0 f_{pM} + c_1 f_{pM+1} + \ldots + c_M f_{(p+1)M}\right) \\ &= \frac{(c_0+c_M)}{M}\bar{h}\sum_{p=0}^{P-1}\left(\frac{f_{pM}}{2} + \frac{f_{(p+1)M}}{2}\right) + \sum_{m=1}^{M-1}\frac{c_m}{M}\bar{h}\sum_{p=0}^{P-1}\left(\frac{f_{pM+m}}{2} + \frac{f_{(p+1)M+m}}{2}\right) \\ &= \sum_{m=0}^{M-1}\alpha_m \bar{h}\sum_{p=0}^{P-1}\left(\frac{f_{m+pM}}{2} + \frac{f_{m+(p+1)M}}{2}\right), \end{aligned} \tag{18}$$

where $\bar{h} = Mh$ denotes the size of the cell clusters. The RHS of (18) is a linear combination of M trapezoidal-type quadratures constructed on a uniform grid of P cells of size $\bar{h} = Mh$. The coefficients of the linear combination are:

$$\alpha_0 = (c_0+c_M)/M, \quad \alpha_1 = c_1/M, \quad \ldots, \quad \alpha_{M-1} = c_{M-1}/M.$$

Moreover, each quadrature with $m > 0$ is a trapezoidal rule shifted by mh, that is, formally it integrates the function f on the interval $[mh, L + mh]$ rather than $[0, L]$. However, as the function f is L-periodic, we obviously have:

$$\int_{mh}^{mh+L} f(x)\,dx = \int_0^L f(x)\,dx. \tag{19}$$

Therefore, we can apply the same argument as used in the proof of Theorem 1 to each individual trapezoidal formula on the RHS of (18). In doing so, we consider the partial sum S_{P-1} and the remainder R_{P-1} of the Fourier series of f. This yields [cf. formula (18)]:

$$\begin{aligned} &h\sum_{p=0}^{P-1}\big(c_0 f_{pM} + c_1 f_{pM+1} + \ldots + c_M f_{(p+1)M}\big)\\ &= \frac{(c_0+c_M)}{M}\int_0^L f(x)\,dx + \sum_{m=1}^{M-1}\frac{c_m}{M}\int_{mh}^{mh+L} f(x)\,dx\\ &+ \sum_{m=0}^{M-1}\alpha_m\bar{h}\sum_{p=0}^{P-1}\left(\frac{R_{P-1}(x_{pM+m})}{2} + \frac{R_{P-1}(x_{(p+1)M+m})}{2}\right). \end{aligned}$$

Then, using equations (16) and (19) we obtain:

$$\begin{aligned} &h\sum_{p=0}^{P-1}\big(c_0 f_{pM} + c_1 f_{pM+1} + \ldots + c_M f_{(p+1)M}\big) - \int_0^L f(x)\,dx\\ &= \sum_{m=0}^{M-1}\alpha_m\bar{h}\sum_{p=0}^{P-1}\left(\frac{R_{P-1}(x_{pM+m})}{2} + \frac{R_{P-1}(x_{(p+1)M+m})}{2}\right). \end{aligned}$$

Finally, the desired estimate (17) is obtained by applying the triangle inequality and estimating the remainder of the Fourier series as:

$$\sup_{0\le x\le L}|R_{P-1}(x)| \le \frac{\zeta_P}{P^{r-1/2}}.$$

This estimate is equivalent to (12) as long as when refining the grid ($N \equiv MP \to \infty$) we keep the order of the quadrature formula M fixed ($M = \text{const}$), while letting the number of clusters P to increase ($P \to \infty$). □

Remark. Note that one of the simplest quadrature formulae, known as the midpoint rule,

$$\int_a^b f(x)\,dx \approx h(f_{1/2} + f_{3/2} + \ldots + f_{N-1/2}), \tag{20}$$

does not formally belong to the class (15). It has accuracy $\mathcal{O}(h^2)$ provided that f'' is bounded, and is obtained by approximating the function f with a constant (zero-degree polynomial) on each grid cell:

$$f(x) \approx Q_0(x, f, x_j, x_{j+1}) = f(x_j + h/2) =: f_{j+1/2}, \quad x \in [x_j, x_{j+1}].$$

Yet the same argument as employed when proving Theorem 2 clearly applies to the quadrature formula (20), which means that the midpoint rule also achieves spectral accuracy when used for integrating smooth periodic functions.

Example. As a numerical demonstration, we calculate the integral

$$\int_0^{2\pi} e^{\sin x}\, dx \tag{21}$$

using Simpson's rule on a sequence of uniform grids with $N = 2, 4, 8, \ldots$ Let us denote by I_N the approximate value of the integral (21) on the grid with N cells. The results obtained with double precision are summarized in Table 1.

TABLE 1
Computation of integral (21) using Simpson's rule.

N	I_N	$\lvert I_N - I_{N/2}\rvert$
2	6.28318530717958712	
4	8.55803615070285417	2.27485084352326705e+00
8	7.94346255032835646	6.14573600374497708e−01
16	7.95492610378320109	1.14635534548446216e−02
32	7.95492652101284392	4.17229642835081904e−07
64	7.95492652101284392	0.0

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