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The superconvergence of composite Newton–Cotes rules for Hadamard finite-part integral on a circle

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Abstract We study the general (composite) Newton–Cotes rules for the computation of Hadamard finite-part integral on a circle with the hypersingular kernel $\sin^{-2}\frac{x-s}{2}$ and focus on their pointwise superconvergence phenomenon, i.e., when the singular point coincides with some a priori known point, the convergence rate is higher than what is globally possible. We show that the superconvergence rate of the (composite) Newton–Cotes rules occurs at the zeros of a special function $\Phi_k(\tau)$ and prove the existence of the superconvergence points. The relation between $\Phi_k(\tau)$ and $\mathcal{S}_k(\tau)$ defined in Wu and Sun (Numer Math 109:143–165, 2008) is established, and the efficient calculation of Cotes coefficients is also discussed. Several numerical examples are provided to validate the theoretical analysis.

Keywords Hadamard finite-part integral · Composite Newton–Cotes rule · Superconvergence · Clausen function

Mathematics Subject Classification (2000) 65D30 · 65D32

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1 Introduction

Consider the following Hadamard finite-part integral

$$I(c, s, f) := \oint_{c}^{c+2\pi} \frac{f(x)}{\sin^2 \frac{x-s}{2}} dx, \quad s \in (c,\ c+2\pi), \tag{1}$$

where $f(x)$ is a 2π-periodic function and c an arbitrary constant. Integral (1) can be defined in a number of ways and those definitions are generally equivalent [29]. Here we take the following definition [31]

$$\oint_{c}^{c+2\pi} \frac{f(x)}{\sin^2 \frac{x-s}{2}} dx = \lim_{\varepsilon \to 0} \left\{ \int_{c}^{s-\varepsilon} \frac{f(x)}{\sin^2 \frac{x-s}{2}} dx + \int_{s+\varepsilon}^{c+2\pi} \frac{f(x)}{\sin^2 \frac{x-s}{2}} dx - \frac{8 f(s)}{\varepsilon} \right\}, \tag{2}$$

$f(x)$ is said to be *finite-part integrable* with respect to the weight $\sin^{-2} \frac{x-s}{2}$ if the limit on the right hand side of (2) exists. A sufficient condition for $f(x)$ to be finite-part integrable is that its first derivative $f'(x)$ is Hölder continuous. This definition implies that $I(c, s, f)$ is a linear operator on f. Throughout this paper, $\oint$ denotes an integral in the Hadamard finite-part sense.

For some boundary value problems (BVP) in unbounded domains, by introducing a circle or an ellipse as an artificial boundary and then by taking derivatives of conventional integral equations on this boundary, integrals of the form (1) occur and some domain decomposition methods as well as certain coupled algorithms can be naturally constructed [5,6,12,14,17,27,30]. Moreover, they also appear frequently in many engineering problems, such as in elasticity, electromagnetic scattering, and so on [13,19]. The efficiency of the boundary element method and many scientific and engineering computational problems often depends on the efficient computation of such integrals.

In recent decades, much attention has been paid to the Hadamard finite-part integrals on the interval of the form:

$$\oint_{a}^{b} \frac{f(x)}{(x-s)^{p+1}} dx := \lim_{\varepsilon \to 0} \left\{ \int_{a}^{s-\varepsilon} \frac{f(x)}{(x-s)^{p+1}} dx + \int_{s+\varepsilon}^{b} \frac{f(x)}{(x-s)^{p+1}} dx - \frac{2 f^{(p)}(s)}{\varepsilon} \right\}, \tag{3}$$
$$s \in (a, b),\ p = 1, 2.$$

Numerous works have been devoted in developing efficient quadrature formulas, such as the Gaussian method [10,16,18,21,22], the Newton–Cotes method [4,15,20, 24–26,28,31,32], the transformation method [2,7,8], the global interpolation method [9,11,13] and so on.

Newton–Cotes rules for evaluating the integral (3) were firstly suggested by Linz [15]. Later, Yu [28] extended this idea to obtain the composite trapezoidal rule for computing (1). It has been shown in their error analysis that one must choose the mesh very carefully such that the singular point is located near the center of a certain subinterval to assure a good accuracy. But in fact, when the singular point s coincides with some a priori known point, Newton–Cotes rules can reach a higher-order convergence rate. This is the so-called *pointwise superconvergence phenomenon* of the Newton–Cotes rules for Hadamard finite-part integrals.

Superconvergence phenomenon of the Newton–Cotes rules was first studied in [24,25] for (3), where the superconvergence rate of the trapezoidal rule and Simpson's rule was presented, respectively. Recently, the superconvergence of the general Newton–Cotes rules for Hadamard finite-part integral (3) with $p = 1$ was studied in Wu and Sun [26]. They proved both theoretically and numerically that the (composite) Newton–Cotes rules can reach the superconvergence rate $O(h^{k+1})$ when the local coordinate of the singular point s is the zero of a certain function $\mathcal{S}_k(\tau)$. In a recent paper [31], we discussed the superconvergence of the trapezoidal rule for evaluating (1). To our knowledge, there is no work about the Newton–Cotes rules with degree higher than one, since the Cotes coefficients of those quadrature formulae are expressed by certain integrals which can not be evaluated analytically. The purpose of this paper is to study the superconvergence, as well as the evaluation of the Cotes coefficients, of arbitrary degree Newton–Cotes rules for Hadamard finite-part integral (1).

Before stating our main idea, some notations and results are introduced, which will be very important in our error analysis. First we recall some ideas in [26]. They defined an function

$$\mathcal{S}_k(\tau) = \psi_k'(\tau) + \sum_{k=1}^{\infty}[\psi_k'(2i+\tau) + \psi_k'(-2i+\tau)], \quad \tau \in (-1, 1), \tag{4}$$

where $\psi_k'(\tau)$ is the first derivative of a function $\psi_k(\tau)$ which is defined as the Hilbert transform of a function

$$\phi_k(\tau) = \prod_{j=0}^{k}(\tau - \tau_j) = \prod_{j=0}^{k}\left(\tau - \frac{2j-k}{k}\right),$$

and showed that the superconverngece phenomenon of composite Newton–Cotes rules for (3) with $p = 1$ occurs when the local coordinate of the singular point s is the zero of the function $\mathcal{S}_k(\tau)$. However, due to the different property of the kernel $\sin^{-2}\frac{x-s}{2}$, the analytic process in [26] cannot be directly applied. Thus, we propose a simple and new analysis technique in this article, which leads to the error expansion as well as the explicit expression of $O(h^k)$ term. Moreover, we show that the superconvergence phenomenon occurs in every subinterval of the partition, while for the composite Newton–Cotes rules for (3), this phenomenon only occurs in those subintervals that are not very close to the endpoints of the integral interval.

Definition 1 The elementary symmetric polynomials are defined as

$$\begin{cases} \sigma_0(x_1, \ldots, x_k) = 1, \\ \sigma_i(x_1, \ldots, x_k) = \sum_{1\le j_1<j_2<\cdots<j_i\le k} x_{j_1}\ldots x_{j_i}, \quad 1 \le i \le k. \end{cases} \tag{5}$$

Moreover, define

$$\sigma_i^k = \sigma_i\left(\frac{1}{k}, \frac{2}{k}, \ldots, \frac{k}{k}\right). \tag{6}$$

Definition 2 [23] Define

$$\begin{cases} \mathrm{S}_n(x) = \sum_{k=1}^{\infty} \dfrac{\sin(kx)}{k^n}, \\ \mathrm{C}_n(x) = \sum_{k=1}^{\infty} \dfrac{\cos(kx)}{k^n}, \end{cases} \tag{7}$$

then the Clausen functions are defined by

$$\mathrm{Cl}_n(x) = \begin{cases} \mathrm{S}_n(x) = \sum_{k=1}^{\infty} \dfrac{\sin(kx)}{k^n}, & n \text{ even}, \\ \mathrm{C}_n(x) = \sum_{k=1}^{\infty} \dfrac{\cos(kx)}{k^n}, & n \text{ odd}. \end{cases} \tag{8}$$

For $n = 1$, the Clausen function takes on the special form

$$\mathrm{Cl}_1(x) = \mathrm{C}_1(x) = -\ln\left|2\sin\frac{x}{2}\right| \tag{9}$$

and for $n = 2$, it becomes Clausen's integral

$$\mathrm{Cl}_2(x) = \mathrm{S}_2(x) = -\int_0^x \ln\left(2\sin\frac{t}{2}\right) dt. \tag{10}$$

The following lemma is followed directly by Definition 2.

Lemma 1 *The Clausen function have some properties as follows*:

(1) *(Recurrence) For any positive integer n, it holds*

$$\mathrm{Cl}'_{n+1}(x) = (-1)^{n+1}\,\mathrm{Cl}_n(x). \tag{11}$$

(2) *(Periodicity) For any integer k, it holds*

$$\mathrm{Cl}_n(x) = \mathrm{Cl}_n(x + 2k\pi). \tag{12}$$

Later, we shall prove that the superconvergence phenomenon occurs at the point s whose local coordinate is the zero of the function

$$\Phi_k(\tau) = \begin{cases} \sum_{i=1}^{k_1} (-1)^{k_1-i} \dfrac{(2k_1-2i+2)!}{(2\pi)^{2k_1-2i+1}} \sigma_{2i-1}^{2k_1}\, \mathrm{Cl}_{2k_1-2i+2}[(1+\tau)\pi], & k = 2k_1; \\ \sum_{i=1}^{k_1} (-1)^{k_1-i} \dfrac{(2k_1-2i+1)!}{(2\pi)^{2k_1-2i}} \sigma_{2i-1}^{2k_1-1}\, \mathrm{Cl}_{2k_1-2i+1}[(1+\tau)\pi], & k = 2k_1 - 1. \end{cases} \tag{13}$$

Since $\Phi_k(\tau)$ is just an expansion of trigonometric series, we can easily prove the existence of the superconvergence points for any integer k. Then, we get an equivalent relation between $\mathcal{S}_k(\tau)$ and $\Phi_k(\tau)$, which reveal the connection between integrals (1) and (3) with $p = 1$, and then show that the local coordinates of the superconvergence points of the (composite) Newton–Cotes rule defined in (16) are the same as those for the corresponding quadrature rule on the interval.

We finish the introduction by outlining the rest of the paper. In the next section, after introducing some basic formulas of the general (composite) Newton–Cotes rules, we present our main result of superconvergence. The complete proof is given in Sect. 3. The existence of superconvergence points and the relation between $\mathcal{S}_k(\tau)$ and $\Phi_k(\tau)$ is established in Sect. 4. In Sect. 5, we discuss the computation of the Cotes coefficients. In Sect. 6, several numerical examples are presented to validate our analysis and concluding remarks are made in the last section.

2 The composite Newton–Cotes rule and its superconvergence for Hadamard finite-part integral (1)

Let $c = x_0 < x_1 < \cdots < x_{n-1} < x_n = c + 2\pi$ be a uniform partition of the interval $[c, c+2\pi]$ with mesh size $h = 2\pi/n$. To define a piecewise Lagrangian interpolation polynomials of degree k, we introduce a further partition in each subinterval,

$$x_i = x_{i0} < x_{i1} < \cdots < x_{ik} = x_{i+1},$$

and a linear transformation

$$x = \hat{x}_i(\tau) := (\tau + 1)(x_{i+1} - x_i)/2 + x_i, \quad \tau \in [-1, 1],$$

from the reference element $[-1, 1]$ to the subinterval $[x_i, x_{i+1}]$. Define the piecewise Lagrangian interpolation polynomial by

$$\mathcal{F}_{kn}(x) = \sum_{j=0}^{k} f(x_{ij}) \frac{l_{ki}(x)}{l'_{ki}(x_{ij})(x - x_{ij})}, \quad x \in [x_i, x_{i+1}], \tag{14}$$

where

$$l_{ki}(x) = \prod_{j=0}^{k} (x - x_{ij}). \tag{15}$$

Replacing $f(x)$ in (1) with $\mathcal{F}_{kn}(x)$, we obtain the general Newton–Cotes rule

$$\mathcal{Q}_{kn}(f)(c, s) = \,=\!\!\!\!\!\!\int_{c}^{c+2\pi} \frac{\mathcal{F}_{kn}(x)}{\sin^2 \frac{x-s}{2}} dx = \sum_{i=0}^{n-1} \sum_{j=0}^{k} \omega_{ij}^{k}(s) f(x_{ij}) = I(c, s, f) - \mathcal{E}_{kn}(f) \tag{16}$$

where $\omega_{ij}^k(s)(0 \le i \le n-1, 0 \le j \le k)$ denote the Cotes coefficients and $\mathcal{E}_{kn}(f)$ the error functional. The computation of the Cotes coefficients $\omega_{ij}^k(s)$ will be discussed in Sect. 5.

For the above quadrature rule, we have the error estimate below.

Theorem 1 *Assume that* $f(x) \in C^{k+\alpha}[c, c+2\pi]$ *and* $f(c) = f(c+2\pi)$. *Let* $\mathcal{Q}_{kn}(f)(c,s)$ *be computed by* (16) *with a uniform mesh. Then, for* $s \ne x_i(0 \le i \le n)$, *there exists a positive constant* C, *independent of* h *and* s, *such that*

$$|\mathcal{E}_{kn}(f)| \le C\gamma^{-1}(h,s)h^{k+\alpha-1}, \tag{17}$$

where

$$\gamma(h,s) = \min_{0\le i\le n} \frac{|s-x_i|}{h}. \tag{18}$$

Proof Let $\mathcal{H}_{kn}(x) = f(x) - \mathcal{F}_{kn}(x)$ and define

$$\kappa_s(x) = \begin{cases} \dfrac{(x-s)^2}{\sin^2\frac{x-s}{2}}, & x \ne s, \\ 4, & x = s. \end{cases} \tag{19}$$

Then, from (16) and (19), we see that

$$\mathcal{E}_{kn}(f) = \fint_c^{c+2\pi} \frac{\mathcal{H}_{kn}(x)}{\sin^2\frac{x-s}{2}}dx = \fint_c^{c+2\pi} \frac{\mathcal{H}_{kn}(x)\kappa_s(x)}{(x-s)^2}dx, \quad s \in (c,\ c+2\pi).$$

Now we split the error into two parts

$$\mathcal{E}_{kn}(f) = 4\fint_c^{c+2\pi} \frac{\mathcal{H}_{kn}(x)}{(x-s)^2}dx + \fint_c^{c+2\pi} \frac{\mathcal{H}_{kn}(x)[\kappa_s(x)-4]}{(x-s)^2}dx. \tag{20}$$

The first part can be directly estimated by Theorem 2.1 in [26], i.e.,

$$\left| \fint_c^{c+2\pi} \frac{\mathcal{H}_{kn}(x)}{(x-s)^2}dx \right| \le C|\ln\gamma(h,s)|h^{k+\alpha-1}. \tag{21}$$

As for the second part, we observe that $[\kappa_s(x)-4](x-s)^{-2}$ is nonnegative and only has a removable discontinuity at $x = s$. So the correspondent finite-part integral degenerates to a Riemann integral and consequently,

$$
\begin{aligned}
\left| \;\ne\!\!\!\!\!\!\int_c^{c+2\pi} \frac{\mathcal{H}_{kn}(x)[\kappa_s(x)-4]}{(x-s)^2}dx \right| &\le \max_{x\in[c,\, c+2\pi]}\{|\mathcal{H}_{kn}(x)|\} \int_c^{c+2\pi} \frac{\kappa_s(x)-4}{(x-s)^2}dx \\
&= \max_{x\in[c,\, c+2\pi]}\{|\mathcal{H}_{kn}(x)|\} \;\ne\!\!\!\!\!\!\int_c^{c+2\pi} \frac{\kappa_s(x)-4}{(x-s)^2}dx \\
&= \max_{x\in[c,\, c+2\pi]}\{|\mathcal{H}_{kn}(x)|\} \left\{ \;\ne\!\!\!\!\!\!\int_c^{c+2\pi} \frac{1}{\sin^2\frac{x-s}{2}}dx - \;\ne\!\!\!\!\!\!\int_c^{c+2\pi} \frac{4}{(x-s)^2}dx \right\} \\
&= \frac{8\pi}{(c+2\pi-s)(s-c)} \max_{x\in[c,\, c+2\pi]}\{|\mathcal{H}_{kn}(x)|\} \\
&\le C\gamma^{-1}(h,s)h^{k+\alpha-1},
\end{aligned}
\tag{22}
$$

where

$$
\;\ne\!\!\!\!\!\!\int_c^{c+2\pi} \frac{1}{\sin^2\frac{x-s}{2}}dx = 0
$$

and the interpolation error estimate

$$
\max_{x\in[c,\, c+2\pi]}\{|\mathcal{H}_{kn}(x)|\} \le Ch^{k+\alpha}
$$

have been used. Now (17) follows from (20)–(22), which completes the proof. □

It is evident that (17) achieves its optimal bound $O(h^{k+\alpha-1})$ when the singular point s is located near the center of a subinterval. However, we find that when s coincides with some special points, the convergence rate can be higher than $O(h^{k+\alpha-1})$. We present the main result in the following theorem and the proof will be given in the next section.

Theorem 2 *Let $\mathcal{Q}_{kn}(f)(c,s)$ be computed by* (16) *with a uniform mesh. Assume that $f(x)$ is periodic with period 2π and τ^* is a zero of $\Phi_k(\tau)$ defined in* (13). *Then there exists a positive constant C, independent of h and s, such that at $s = \hat{x}_i(\tau^*)$*

$$
|\mathcal{E}_{kn}(f)| \le \begin{cases} Ch^{k+\alpha}, & f(x) \in C^{k+1+\alpha}(c, c+2\pi), \\ C|\ln h|h^{k+1}, & f(x) \in C^{k+2}(c, c+2\pi), \end{cases}
\tag{23}
$$

where $0 < \alpha < 1$.

By comparing Theorem 2 with Theorem 1, we can see that the convergence rate of the composite Newton–Cotes rules at certain points is one order higher than that at other points. Besides, by an identity which will be illustrated in Sect. 4, we can easily see that the zeros of $\Phi_k(\tau)$ are the same as those of $\mathcal{S}_k(\tau)$, defined in (4). More interesting is that in these cases the superconvergence points locate in every subinterval of the partition, which is different from the result in [26].

3 The proof of Theorem 2

Assume that $s \in (x_m, x_{m+1})$ for some m and let $s = x_m + (1+\tau)h/2$ with $\tau \in (-1, 1)$ denoting its local coordinate. Define

$$e_{ij}^k(x) = \sigma_j(x - x_{i0}, x - x_{i1}, \ldots, x - x_{ik}), \quad 0 \le i \le n-1, 0 \le j \le k+1. \tag{24}$$

Lemma 2 *Let the function $e_{ij}^k(x)$ be defined by (24), then, for any integer k, we have*

$$\begin{cases} {e_{i,k+1}^k}'(x) = e_{ik}^k(x), \\ {e_{ik}^k}'(x) = 2e_{i,k-1}^k(x), \\ \cdots \\ {e_{i1}^k}'(x) = (k+1)e_{i0}^k(x) \end{cases} \tag{25}$$

and

$$\begin{cases} e_{ij}^k(x_{i+1}) = \sigma_j^k h^j, \\ e_{ij}^k(x_i) = (-1)^j \sigma_j^k h^j, \end{cases} \tag{26}$$

where $0 \le i \le n-1, 0 \le j \le k+1$.

Proof (25) can be obtained by taking the derivatives of $e_{ij}^k(x_{i+1})$, $1 \le j \le k+1$ and noting definitions of σ_i and $e_{ij}^k(x)$, given in (5) and (24), respectively. (26) is directly followed by (5), (6) and (24). □

Define

$$\oint_{x_m}^{x_{m+1}} \frac{f(x)}{\sin^2 \frac{x-s}{2}} dx = \lim_{\varepsilon \to 0} \left\{ \int_{x_m}^{s-\varepsilon} \frac{f(x)}{\sin^2 \frac{x-s}{2}} dx + \int_{s+\varepsilon}^{x_{m+1}} \frac{f(x)}{\sin^2 \frac{x-s}{2}} dx - \frac{8f(s)}{\varepsilon} \right\} \tag{27}$$

and

$$\mathcal{I}_{n,i}^k(s) = \begin{cases} \displaystyle\int_{x_i}^{x_{i+1}} \frac{\prod_{j=0}^k (x - x_{ij})}{\sin^2 \frac{x-s}{2}} dx, & i \ne m, \\ \displaystyle\oint_{x_m}^{x_{m+1}} \frac{\prod_{j=0}^k (x - x_{mj})}{\sin^2 \frac{x-s}{2}} dx, & i = m. \end{cases} \tag{28}$$

Lemma 3 *Assume $s = x_m + (\tau + 1)h/2$ with $\tau \in (-1, 1)$. Let $\mathcal{I}^k_{n,i}(s)$ be defined by (28), then we have*

$$\mathcal{I}^k_{n,i}(s) = -4\sum_{j=0}^{k}(-1)^{[\frac{k-j+1}{2}]}(k-j+1)!\sigma^k_j h^j \times[\mathrm{Cl}_{k-j+1}(x_{i+1}-s) + (-1)^{j+1}\,\mathrm{Cl}_{k-j+1}(x_i - s)], \tag{29}$$

where $\{\sigma^k_j\}^k_{j=0}$ are defined in (6).

Proof For $i = m$, by the definition (2), some integrations by parts and Lemma 2, we have

$$\begin{aligned}\mathcal{I}^k_{n,m}(s) &= \lim_{\epsilon\to 0}\left\{\left(\int_{x_m}^{s-\epsilon} + \int_{s+\epsilon}^{x_{m+1}}\right)\frac{\prod_{j=0}^k (x-x_{mj})}{\sin^2\frac{x-s}{2}}dx - \frac{8\prod_{j=0}^k (s-x_{mj})}{\epsilon}\right\}\\ &= \lim_{\epsilon\to 0}\left\{2\left(\int_{x_m}^{s-\epsilon} + \int_{s+\epsilon}^{x_{m+1}}\right)e^k_{mk}(x)\cot\frac{x-s}{2}dx\right\}\\ &= 4h^k\sigma^k_k\left(\ln\left|\sin\frac{x_{m+1}-s}{2}\right| - (-1)^k\ln\left|\sin\frac{x_m - s}{2}\right|\right)\\ &\quad - 8\int_{x_m}^{x_{m+1}}\ln\left|\sin\frac{x-s}{2}\right| e^k_{m,k-1}(x)\,dx.\end{aligned} \tag{30}$$

For $i \neq m$, taking integration by parts on the correspondent Riemann integral, we have

$$\mathcal{I}^k_{n,i}(s) = 4h^k\sigma^k_k\left(\ln\left|\sin\frac{x_{i+1}-s}{2}\right| - (-1)^k\ln\left|\sin\frac{x_i - s}{2}\right|\right) - 8\int_{x_i}^{x_{i+1}}\ln\left|\sin\frac{x-s}{2}\right| e^k_{i,k-1}(x)\,dx. \tag{31}$$

By the property (26) of $e^k_{i,k-1}(x)$, we can easily obtain

$$\int_{x_i}^{x_{i+1}} e^k_{i,k-1}(x)dx = \frac{[e^k_{i,k}(x_{i+1}) - e^k_{i,k}(x_i)]}{2} = \frac{1-(-1)^k}{2}\sigma^k_k h^k. \tag{32}$$

If k is even,

$$\mathcal{I}_{n,i}^{k}(s) = 4h^k\sigma_k^k\left(\ln\left|2\sin\frac{x_{i+1}-s}{2}\right| - \ln\left|2\sin\frac{x_i-s}{2}\right|\right)$$
$$-8\int_{x_i}^{x_{i+1}}\ln\left|2\sin\frac{x-s}{2}\right| e_{i,k-1}^k(x)\,dx + 8\ln 2\int_{x_i}^{x_{i+1}} e_{i,k-1}^k(x)\,dx$$
$$= -4h^k\sigma_k^k\left[\mathrm{Cl}_1(x_{i+1}-s)-\mathrm{Cl}_1(x_i-s)\right]+8\int_{x_i}^{x_{i+1}}\mathrm{Cl}_1(x-s)e_{i,k-1}^k(x)\,dx; \quad (33)$$

if k is odd,

$$\mathcal{I}_{n,i}^{k}(s) = 4h^k\sigma_k^k\left(\ln\left|2\sin\frac{x_{i+1}-s}{2}\right| + \ln\left|2\sin\frac{x_i-s}{2}\right|\right)$$
$$-8\int_{x_i}^{x_{i+1}}\ln\left|2\sin\frac{x-s}{2}\right| e_{i,k-1}^k(x)\,dx - 8\ln 2\left(h^k\sigma_k^k - \int_{x_i}^{x_{i+1}} e_{i,k-1}^k(x)\,dx\right)$$
$$= -4h^k\sigma_k^k\left[\mathrm{Cl}_1(x_{i+1}-s)+\mathrm{Cl}_1(x_i-s)\right]+8\int_{x_i}^{x_{i+1}}\mathrm{Cl}_1(x-s)e_{i,k-1}^k(x)\,dx, \quad (34)$$

where (9) and (32) have been used.

Then, by taking integration by parts, Lemmas 1 and 2, we get

$$\int_{x_i}^{x_{i+1}}\mathrm{Cl}_j(x-s)e_{i,k-j}^k(x)\,dx$$
$$= (-1)^{j+1}\sigma_{k-j}^k h^{k-j}[\mathrm{Cl}_{j+1}(x_{i+1}-s) + (-1)^{k-j+1}\mathrm{Cl}_{j+1}(x_i-s)]$$
$$-(-1)^{j+1}(j+2)\int_{x_i}^{x_{i+1}}\mathrm{Cl}_{j+1}(x-s)e_{i,k-j-1}^k(x)\,dx, \quad j=1,\ldots,k-1, \quad (35)$$

and thus, (29) is followed by repeated use of integration by parts for (33) and (34), together with (35) from $j=1$ to $j=k-1$. The proof is completed. □

Lemma 4 *Under the same assumptions of Lemma 3, we have*

$$\sum_{i=1}^{n}\mathcal{I}_{n,i}^{k}(s) = -8h^k\Phi_k(\tau), \quad (36)$$

where $\Phi_k(\tau)$ is defined in (13).

Proof By (29), if $k = 2k_1 - 1$, we have

$$\sum_{i=0}^{n-1} \mathcal{I}_{n,i}^{k}(s) = -4 \sum_{j=0}^{k} (-1)^{[\frac{k-j+1}{2}]} (k-j+1)! \sigma_j^k h^j \times \sum_{i=0}^{n-1} \Big[\mathrm{Cl}_{k-j+1}(x_{i+1}-s) + (-1)^{j+1} \mathrm{Cl}_{k-j+1}(x_i - s) \Big]$$
$$= -8 \sum_{j=1}^{k_1} (-1)^{k_1-j} (2k_1 - 2j + 1)! \sigma_{2j-1}^{2k_1-1} h^{2j-1} \sum_{i=0}^{n-1} \mathrm{Cl}_{2k_1-2j+1}(x_{i+1}-s)$$
$$= -8 \sum_{j=1}^{k_1} (-1)^{k_1-j} (2k_1 - 2j + 1)! \sigma_{2j-1}^{2k_1-1} h^{2j-1} \frac{1}{n^{2k_1-2j}} \mathrm{Cl}_{2k_1-2j+1}[n(x_1 - s)]$$
$$= -8h^{2k_1-1} \sum_{j=1}^{k_1} (-1)^{k_1-j} \frac{(2k_1-2j+1)!}{(2\pi)^{2k_1-2j}} \sigma_{2j-1}^{2k_1-1} \mathrm{Cl}_{2k_1-2j+1}[(1+\tau)\pi];$$

if $k = 2k_1$, we have

$$\sum_{i=0}^{n-1} \mathcal{I}_{n,i}^{k}(s) = -4 \sum_{j=0}^{k} (-1)^{[\frac{k-j+1}{2}]} (k-j+1)! \sigma_j^k h^j \times \sum_{i=0}^{n-1} \Big[\mathrm{Cl}_{k-j+1}(x_{i+1}-s) + (-1)^{j+1} \mathrm{Cl}_{k-j+1}(x_i - s) \Big]$$
$$= -8 \sum_{j=1}^{k_1} (-1)^{k_1-j+1} (2k_1 - 2j + 2)! \sigma_{2j-1}^{2k_1} h^{2j-1} \sum_{i=0}^{n-1} \mathrm{Cl}_{2k_1-2j+2}(x_{i+1}-s)$$
$$= -8 \sum_{j=1}^{k_1} (-1)^{k_1-j+1} (2k_1 - 2j + 2)! \sigma_{2j-1}^{2k_1} h^{2j-1} \frac{1}{n^{2k_1-2j+1}} \mathrm{Cl}_{2k_1-2j+2}[n(x_1 - s)]$$
$$= 8h^{2k_1} \sum_{j=1}^{k_1} (-1)^{k_1-j} \frac{(2k_1-2j+2)!}{(2\pi)^{2k_1-2j+1}} \sigma_{2j-1}^{2k_1} \mathrm{Cl}_{2k_1-2j+2}[(1+\tau)\pi],$$

where

$$\sum_{i=0}^{n-1} \cos[k(x_{i+1}-s)] = \begin{cases} n\cos[k(x_1 - s)], & k = nj, \\ 0, & \text{else} \end{cases}$$

and

$$\sum_{i=0}^{n-1} \sin[k(x_{i+1} - s)] = \begin{cases} n\sin[k(x_1 - s)], & k = nj, \\ 0, & \text{else} \end{cases}$$

have been used. The proof is completed. □

Lemma 5 *Under the same assumptions of Lemma 3, we have*

$$\left| \sum_{i=0, i\neq m}^{n-1} \int_{x_i}^{x_{i+1}} \frac{f^{(k+1)}(\xi_i) - f^{(k+1)}(s)}{(k+1)! \sin^2 \frac{x-s}{2}} l_{ki}(x)\, dx \right| \leq \begin{cases} C\varrho(h, s, c)h^{k+\alpha}, & f(x) \in C^{k+1+\alpha}[c, c+2\pi], \\ C\varrho(h, s, c)h^{k+1}|\ln h|, & f(x) \in C^{k+2}[c, c+2\pi], \end{cases} \tag{37}$$

where $\xi_i \in [x_i, x_{i+1}]$*,* $0 < \alpha < 1$*,*

$$\varrho(h, s, c) = \max_{c \leq x \leq c+2\pi} \{\kappa_s(x)\} \gamma^{-2}(h, s). \tag{38}$$

and $l_{ki}(x)$ *is defined in* (15).

Proof For $i \neq m$, we get

$$\int_{x_i}^{x_{i+1}} \frac{|l_{ki}(x)|}{\sin^2 \frac{x-s}{2}} dx \leq h^{k-1} \int_{x_i}^{x_{i+1}} \frac{(x - x_i)(x_{i+1} - x)}{\sin^2 \frac{x-s}{2}} dx,$$

where

$$\int_{x_i}^{x_{i+1}} \frac{(x - x_i)(x_{i+1} - x)}{\sin^2 \frac{x-s}{2}} dx = -4h \ln \left| \sin \frac{x_{i+1} - s}{2} \sin \frac{x_i - s}{2} \right| + 8 \int_{x_i}^{x_{i+1}} \ln \left| \sin \frac{x-s}{2} \right| dx, \quad i \neq m$$

is actually the error of the trapezoidal rule for certain Riemann integral on $[x_i, x_{i+1}]$. Thus, there exists $\tilde{x}_i \in (x_i, x_{i+1})$, $i \neq m$, such that

$$\int_{x_i}^{x_{i+1}} \frac{|l_{ki}(x)|}{\sin^2 \frac{x-s}{2}} dx \leq \frac{h^{k+2}}{6 \sin^2 \frac{\tilde{x}_i - s}{2}}.$$

Then, by the above formula and the first mean value theorem for integration, we get

$$
\begin{aligned}
&\left| \sum_{i=0, i\neq m}^{n-1} \int_{x_i}^{x_{i+1}} \frac{f^{(k+1)}(\xi_i) - f^{(k+1)}(s)}{(k+1)! \sin^2 \frac{x-s}{2}} l_{ki}(x)\, dx \right| \\
&\leq \sum_{i=0, i\neq m}^{n-1} \int_{x_i}^{x_{i+1}} \frac{|f^{(k+1)}(\xi_i) - f^{(k+1)}(s)|}{(k+1)! \sin^2 \frac{x-s}{2}} |l_{ki}(x)|\, dx \\
&\leq \sum_{i=0, i\neq m}^{n-1} \frac{|f^{(k+1)}(\eta_i) - f^{(k+1)}(s)|}{(k+1)!} \int_{x_i}^{x_{i+1}} \frac{|l_{ki}(x)|}{\sin^2 \frac{x-s}{2}}\, dx \\
&\leq \sum_{i=0, i\neq m}^{n-1} \frac{C h^{k+2} |\eta_i - s|^\alpha}{6(k+1)!(\tilde{x}_i - s)^2} \frac{(\tilde{x}_i - s)^2}{\sin^2 \frac{\tilde{x}_i - s}{2}} \\
&\leq C \max_{c\leq x\leq c+2\pi} \{\kappa_s(x)\} \left[\sum_{i=0}^{m-1} \frac{h^{k+2}|x_i - s|^\alpha}{6(k+1)!(x_{i+1}-s)^2} + \sum_{i=m+1}^{n-1} \frac{h^{k+2}|x_{i+1}-s|^\alpha}{6(k+1)!(x_i - s)^2} \right],
\end{aligned}
\tag{39}
$$

where $\eta_i \in [x_i, x_{i+1}]$ and $\kappa_s(x)$ is defined in (19). Noting $s = x_m + (\tau+1)h/2 (-1 < \tau < 1)$, we have

$$
\begin{aligned}
\sum_{i=0}^{m-1} \frac{h^{k+2}|x_i - s|^\alpha}{6(k+1)!(x_{i+1}-s)^2} &\leq \sum_{i=0}^{m-1} \frac{h^{k+2+\alpha} + h^{k+2}|x_{i+1} - s|^\alpha}{6(k+1)!(x_{i+1}-s)^2} \\
&\leq \frac{h^{k+\alpha}}{6(k+1)!} \sum_{i=0}^{m-1} \frac{1 + |i - m + 1 - \frac{1+\tau}{2}|^\alpha}{(i - m + 1 - \frac{1+\tau}{2})^2} \\
&\leq \begin{cases} \dfrac{Ch^{k+\alpha}}{(1+\tau)^2}, & 0 < \alpha < 1, \\[2ex] \dfrac{Ch^{k+1}|\ln h|}{(1+\tau)^2}, & \alpha = 1. \end{cases}
\end{aligned}
\tag{40}
$$

Similarly,

$$
\sum_{i=m+1}^{n-1} \frac{h^{k+2}|x_{i+1} - s|^\alpha}{6(k+1)!(x_i - s)^2} \leq \begin{cases} \dfrac{Ch^{k+\alpha}}{(1-\tau)^2}, & 0 < \alpha < 1, \\[2ex] \dfrac{Ch^{k+1}|\ln h|}{(1-\tau)^2}, & \alpha = 1. \end{cases}
\tag{41}
$$

Now putting (39)–(41) together and making use of (18) yields (37), which completes the proof. □

Lemma 6 *Assume $f(c) = f(c+2\pi)$ and let $Q_{kn}(f)(c,s)$ be computed by (16) with a uniform mesh. Then*

$$\mathcal{E}_{kn}(f) = -\frac{8f^{(k+1)}(s)}{(k+1)!}h^k\Phi_k(\tau) + \mathcal{R}_k(s), \tag{42}$$

where

$$|\mathcal{R}_k(s)| \le \begin{cases} C\varrho(h,s,c)h^{k+\alpha}, & f(x) \in C^{k+1+\alpha}[c, c+2\pi], \\ C\varrho(h,s,c)h^{k+1}|\ln h|, & f(x) \in C^{k+2}[c, c+2\pi], \end{cases} \tag{43}$$

and $0 < \alpha < 1$.

Proof Firstly, we recall from the property of Lagrangian interpolation that, there exists $\xi_i \in (x_i, x_{i+1})$, which may depend upon x, such that

$$\mathcal{H}_{kn}(x) = \frac{f^{(k+1)}(\xi_i)}{(k+1)!}(x - x_{i0})\cdots(x - x_{ik}), \quad x \in [x_i, x_{i+1}].$$

Then, by Lemma 4, we have

$$\begin{aligned} \left(\int_c^{x_m} + \int_{x_{m+1}}^{c+2\pi}\right)\frac{\mathcal{H}_{kn}(x)}{\sin^2\frac{x-s}{2}}dx &= \sum_{i=0,i\neq m}^{n-1}\int_{x_i}^{x_{i+1}}\frac{f^{(k+1)}(\xi_i) - f^{(k+1)}(s)}{(k+1)!\sin^2\frac{x-s}{2}}l_{ki}(x)\,dx \\ &\quad - \frac{f^{(k+1)}(s)}{(k+1)!}\mathcal{I}^k_{n,m}(s) + \frac{f^{(k+1)}(s)}{(k+1)!}\sum_{i=0}^{n-1}\mathcal{I}^k_{n,i}(s) \\ &= \sum_{i=0,i\neq m}^{n-1}\int_{x_i}^{x_{i+1}}\frac{f^{(k+1)}(\xi_i) - f^{(k+1)}(s)}{(k+1)!\sin^2\frac{x-s}{2}}l_{ki}(x)\,dx \\ &\quad - \frac{f^{(k+1)}(s)}{(k+1)!}\mathcal{I}^k_{n,m}(s) - \frac{8f^{(k+1)}(s)}{(k+1)!}h^k\Phi_k(\tau). \end{aligned} \tag{44}$$

Secondly, by setting

$$\mathcal{E}_m(x) = f(x) - \mathcal{F}_{kn}(x) - \frac{f^{(k+1)}(s)}{(k+1)!}(x - x_{m0})\cdots(x - x_{mk}), \; x \in [x_m, x_{m+1}]$$

and through a similar derivation of (20), we get

$$\begin{aligned} \fint_{x_m}^{x_{m+1}}\frac{\mathcal{H}_{kn}(x)}{\sin^2\frac{x-s}{2}}dx &= \fint_{x_m}^{x_{m+1}}\frac{\mathcal{E}_m(x)}{\sin^2\frac{x-s}{2}}dx + \frac{f^{(k+1)}(s)}{(k+1)!}\mathcal{I}^k_{n,m}(s) \\ &= 4\fint_{x_m}^{x_{m+1}}\frac{\mathcal{E}_m(x)}{(x-s)^2}dx + \fint_{x_m}^{x_{m+1}}\frac{\mathcal{E}_m(x)[\kappa_s(x) - 4]}{(x-s)^2}dx \\ &\quad + \frac{f^{(k+1)}(s)}{(k+1)!}\mathcal{I}^k_{n,m}(s). \end{aligned} \tag{45}$$

Putting (44) and (45) together yields (42) with

$$\mathcal{R}_k(s) = 4\mathcal{R}_k^{(1)}(s) + \mathcal{R}_k^{(2)}(s) + \mathcal{R}_k^{(3)}(s), \quad \mathcal{R}_k^{(1)}(s) = \oint_{x_m}^{x_{m+1}} \frac{\mathcal{E}_m(x)}{(x-s)^2}dx,$$

$$\mathcal{R}_k^{(2)}(s) = \oint_{x_m}^{x_{m+1}} \frac{\mathcal{E}_m(x)[\kappa_s(x)-4]}{(x-s)^2}dx,$$

$$\mathcal{R}_k^{(3)}(s) = \sum_{i=0,i\neq m}^{n-1} \int_{x_i}^{x_{i+1}} \frac{f^{(k+1)}(\xi_i) - f^{(k+1)}(s)}{(k+1)!\sin^2\frac{x-s}{2}} l_{ki}(x)\,dx.$$

Now we estimate $\mathcal{R}_k(s)$ term by term. Note that $f(x) \in C^{k+1+\alpha}[c, c+2\pi](0 < \alpha \leq 1)$ implies

$$|\mathcal{E}_m^{(i)}(x)| \leq Ch^{k+1+\alpha-i}, \quad i = 0, 1, 2.$$

Then, by using the identity (cf.[20])

$$\oint_a^b \frac{f(x)}{(x-s)^2}dx = \frac{(b-a)f(s)}{(b-s)(s-a)} + f'(s)\ln\frac{b-s}{s-a} + \int_a^b \frac{f(x)-f(s)-f'(s)(x-s)}{(x-s)^2}dx,$$

we have

$$|\mathcal{R}_k^{(1)}(s)| \leq \left|\frac{h\mathcal{E}_m(s)}{(x_{m+1}-s)(s-x_m)}\right| + \left|\mathcal{E}_m'(s)\ln\frac{x_{m+1}-s}{s-x_m}\right| + \left|\int_{x_m}^{x_{m+1}} \frac{1}{2}\mathcal{E}_m''(\sigma(x))dx\right|$$
$$\leq C\gamma^{-1}(h,s)h^{k+\alpha},$$

where $\sigma(x) \in (x_m, x_{m+1})$. As for the second term, by an argument similar to that of (22), we see that

$$\left|\mathcal{R}_k^{(2)}(s)\right| \leq \max|\mathcal{E}_m(x)| \int_{x_m}^{x_{m+1}} \frac{\kappa_s(x)-4}{(x-s)^2}dx$$
$$= \max|\mathcal{E}_m(x)| \oint_{x_m}^{x_{m+1}} \frac{\kappa_s(x)-4}{(x-s)^2}dx$$

$$
\begin{aligned}
&= \max|\mathcal{E}_m(x)| \left\{ \int\!\!\!\!\!\!=_{x_m}^{x_{m+1}} \frac{1}{\sin^2\frac{x-s}{2}} dx - \int\!\!\!\!\!\!=_{x_m}^{x_{m+1}} \frac{4}{(x-s)^2} dx \right\} \\
&= \max|\mathcal{E}_m(x)| \left\{ -2\cot\frac{s-x_m}{2} - 2\cot\frac{x_{m+1}-s}{2} + \frac{4h}{(x_{m+1}-s)(s-x_m)} \right\} \\
&\le C\gamma^{-1}(h,s)h^{k+\alpha}.
\end{aligned}
$$

The third term $\mathcal{R}_k^{(3)}(s)$ can be estimated directly by Lemma 5. Putting above estimates together leads to (43), which completes the proof. □

We must point out that, in Lemma 6, we actually obtain the error expansion of the composite Newton–Cotes rules (16) and moreover, get the explicit expression of the term of $O(h^k)$. Thanks to this error expansion, the finding and the proof of the existence of the superconvergence points become very easy, which is quite different from the case where finite-part integral on the interval with $p = 1$ is involved (cf. [24,25]). Besides, if $k+1$-order derivatives of $f(x)$ at s can be evaluated, then by adding the first term in the right hand side of (42) into the composite Newton–Cotes rule (16), a modified composite Newton–Cotes rule with approximate $k+1$-order accuracy is obtained.

The following lemma will be used in the proof of Theorem 2, which has been obtained in [31].

Lemma 7 *Assume that $f(x)$ is a periodic function with period 2π. Assume further that $f(x)$ is finite-part integrable with respect to the weight $\sin^{-2}\frac{x-s}{2}$. Then*

$$
\int\!\!\!\!\!\!=_{c}^{c+2\pi} \frac{f(x)}{\sin^2\frac{x-s}{2}} dx = \int\!\!\!\!\!\!=_{\tilde{c}}^{\tilde{c}+2\pi} \frac{f(x)}{\sin^2\frac{x-s}{2}} dx, \tag{46}
$$

holds for any $s \in (c,\ c+2\pi)$ and $\tilde{c} \in (s-2\pi, s)$.

The proof of Theorem 2 Recall that $\mathcal{F}_{kn}(x)$, defined by (14), is the Lagrangian interpolation of $f(x)$ on $[c, c+2\pi]$. We extend $\mathcal{F}_{kn}(x)$ to $(-\infty,\infty)$ to obtain a 2π-periodic function and denote the resulting function still by $\mathcal{F}_{kn}(x)$. Clearly, $\mathcal{F}_{kn}(x)$ becomes the Lagrangian interpolation of $f(x)$ on $(-\infty,+\infty)$. By Lemma 7, for any $s = x_m + (\tau+1)h/2(-1 < \tau < 1,\ 0 \le m \le n-1)$ and $\tilde{c} \in (s-2\pi, s)$, we have

$$
\mathcal{E}_{kn}(f)(c,s) = \mathcal{E}_{kn}(f)(\tilde{c},s). \tag{47}
$$

We first consider the case where $m > [n/2]$ and choose $\tilde{c} = x_{m-[n/2]}$. Let $\tilde{c} = \tilde{x}_0 < \tilde{x}_1 < \cdots < \tilde{x}_{n-1} < \tilde{x}_n = \tilde{c}+2\pi$ be a uniform partition of $[\tilde{c},\ \tilde{c}+2\pi]$ with mesh size h. It is evident that $\mathcal{F}_{kn}(x)$ is still the Lagrangian interpolation of $f(x)$ on this new partition and consequently, the result of Lemma 6 holds, which leads to

$$
\mathcal{E}_{kn}(f)(\tilde{c},s) = -\frac{8f^{(k+1)}(s)}{(k+1)!}h^k\Phi_k(\tau) + \mathcal{R}_k(s), \tag{48}
$$

where

$$|\mathcal{R}_k(s)| \le \begin{cases} C\varrho(h,s,\tilde{c})h^{k+\alpha}, & f(x)\in C^{k+1+\alpha}[\tilde{c},\tilde{c}+2\pi],\ 0<\alpha<1, \\ C\varrho(h,s,\tilde{c})h^{k+1}|\ln h|, & f(x)\in C^{k+2}[\tilde{c},\tilde{c}+2\pi] \end{cases} \tag{49}$$

with $\varrho(h,s,\tilde{c})$ defined by (38). Now, by the assumption $s = x_m + \frac{1+\tau^*}{2}h$, we find that

$$s = \tilde{x}_{[n/2]} + \frac{1+\tau^*}{2}h, \tag{50}$$

which implies that the local coordinate of s is $\tau = \tau^*$, where τ^* is the zero of (13). Then we are led to the results that the first term in the right hand side of (48) vanishes and moreover, $\gamma(h,s)$ is bounded by (18). Therefore, from (18), (38) and (50), we deduce that

$$\varrho(h,s,\tilde{c}) \le C.$$

Incorporating this result with (48) and (49) yields

$$|\mathcal{E}_{kn}(f)(\tilde{c},s)| \le \begin{cases} Ch^{k+\alpha}, & f(x)\in C^{p+1+\alpha}[\tilde{c},\tilde{c}+2\pi],\ 0<\alpha<1, \\ Ch^{k+1}|\ln h|, & f(x)\in C^{k+2}[\tilde{c},\tilde{c}+2\pi]. \end{cases}$$

Now (23) follows directly from (47).

At last, we suggest the modified composite Newton–Cotes rule aforementioned, denoting by $\tilde{\mathcal{Q}}_{kn}(f)(c,s)$, defined by

$$\tilde{\mathcal{Q}}_{kn}(f)(c,s) = \mathcal{Q}_{kn}(f)(c,s) - \frac{8f^{(k+1)}(s)}{(k+1)!}h^k\Phi_k(\tau) \tag{51}$$

We conclude this section by the following theorem, whose proof is a natural consequence of Theorem 2.

Theorem 3 *Let $\tilde{\mathcal{Q}}_{kn}(f)(c,s)$ be computed by (51) with a uniform mesh, and assume that $f(x)$ is periodic with period 2π, then there exists a positive constant C, independent of h and s, such that*

$$|I(c,s,f)-\tilde{\mathcal{Q}}_{kn}(f)(c,s)| \le \begin{cases} C\varrho(h,s,c)h^{k+\alpha}, & f(x)\in C^{k+1+\alpha}[c,c+2\pi], \\ C\varrho(h,s,c)h^{k+1}|\ln h|, & f(x)\in C^{k+2}[c,c+2\pi] \end{cases} \tag{52}$$

where $0<\alpha<1$.

Remark When $k=1$, $\mathcal{Q}_{1n}(f)(c,s)$ is actually the trapezoidal rule, and the $O(h)$ term can be represented as

$$-4hf''(s)\Phi_1(\tau) = 4hf''(s)\ln\left(2\cos\frac{\tau\pi}{2}\right),$$

which coincide with the result in [31].

4 The existence of superconvergence points

We observe from (48) and (49) that, the first order term vanishes if and only if $\tau = \tau^*$, and thus we can get the superconvergence of the composite Newton–Cotes rules at these points. A natural question raised is whether the zero τ^* of the function $\Phi_k(\tau)$ exists.

Theorem 4 *For any positive k, the function $\Phi_k(\tau)$, defined by (13), has at least one zero in $(-1, 1)$.*

Proof When k is even, it's obvious that $\tau^* = 0$ is one zero of $\Phi_k(\tau)$. What remains is only to consider the case k is odd. Let $k = 2k_1 - 1$ and $\Psi_k(\tau)$ be the function of τ, defined by

$$\Psi_k(\tau) = \sum_{i=1}^{k_1} (-1)^{k_1-i} \frac{(2k_1 - 2i + 1)!}{(2\pi)^{2k_1-2i}} \sigma_{2i-1}^{2k_1-1} \operatorname{Cl}_{2k_1-2i+2}[(1 + \tau)\pi]. \tag{53}$$

From Definition 2, it is easy to see that $\Psi_k(\tau)$ vanishes at $\tau = 0$ for odd k. Moreover,

$$\lim_{\tau \to 1-} \Psi_k(\tau) = 0.$$

By Rolle's theorem, the first derivative of $\Psi_k(\tau)$ has at least one zero in $(0, 1)$. On the other hand, by (13) and (53), we find that for odd k,

$$\Psi_k'(\tau) = \Phi_k(\tau).$$

As a result, $\Phi_k(\tau)$ has at least one zero in $(0, 1)$ when k is odd. □

Now we establish the relation between $\mathcal{S}_k(\tau)$ and $\Phi_k(\tau)$.

Lemma 8 (Lemma 3.3, [26]) *Assume $s = x_m + (1 + \tau)h/2$ for some m and let $c_i = 2(s - x_i)/h - 1 = 2(m - i) + \tau$, $0 \le i \le n - 1$. Then, we have*

$$-\frac{h^k}{2^{k-1}} \psi_k'(2(m-i)+\tau) = -\frac{h^k}{2^{k-1}} \psi_k'(c_i) = \begin{cases} \displaystyle ⨎_{x_i}^{x_{i+1}} \frac{1}{(x - s)^2} \prod_{j=0}^{k} (x - x_{ij})\, dx, & i = m, \\ \displaystyle \int_{x_i}^{x_{i+1}} \frac{1}{(x - s)^2} \prod_{j=0}^{k} (x - x_{ij})\, dx, & i \ne m. \end{cases}$$

Theorem 5 *Under the assumption of Lemma 8, let $\Phi_k(\tau)$ and $\mathcal{S}_k(\tau)$ be defined in (13) and (4), respectively. Then*

$$\Phi_k(\tau) = \frac{1}{2^k} \mathcal{S}_k(\tau). \tag{54}$$

Proof By using the equality [1]

$$\frac{\pi^2}{\sin^2 \pi x} = \sum_{l=-\infty}^{\infty} \frac{1}{(x + l)^2},$$

we can easily get

$$\frac{1}{\sin^2\frac{x-s}{2}} = \frac{4}{(x-s)^2} + \sum_{l=1}^{\infty}\frac{4}{(x-s+2l\pi)^2} + \sum_{l=1}^{\infty}\frac{4}{(x-s-2l\pi)^2}. \tag{55}$$

Noting that

$$\begin{aligned}
&\;\;\;\;\;\;\;\;\;\;\;\; \neq\!\!\!\!\!\!\int_{x_m}^{x_{m+1}} \frac{\prod_{j=0}^{k}(x-x_{mj})}{\sin^2\frac{x-s}{2}}dx\\
&= \lim_{\epsilon\to\infty}\left\{\left(\int_{x_m}^{s-\epsilon}+\int_{s+\epsilon}^{x_{m+1}}\right)\frac{\prod_{j=0}^{k}(x-x_{mj})}{\sin^2\frac{x-s}{2}}dx - \frac{8\prod_{j=0}^{k}(s-x_{mj})}{\epsilon}\right\}\\
&= 4\lim_{\epsilon\to\infty}\left\{\left(\int_{x_m}^{s-\epsilon}+\int_{s+\epsilon}^{x_{m+1}}\right)\frac{\prod_{j=0}^{k}(x-x_{mj})}{(x-s)^2}dx - \frac{2\prod_{j=0}^{k}(s-x_{mj})}{\epsilon}\right\}\\
&\quad + 4\sum_{l=1}^{\infty}\int_{x_m}^{x_{m+1}}\frac{\prod_{j=0}^{k}(x-x_{mj})}{(x-s+2l\pi)^2}\,dx + 4\sum_{l=1}^{\infty}\int_{x_m}^{x_{m+1}}\frac{\prod_{j=0}^{k}(x-x_{mj})}{(x-s-2l\pi)^2}\,dx\\
&= 4\,\neq\!\!\!\!\!\!\int_{x_m}^{x_{m+1}}\frac{\prod_{j=0}^{k}(x-x_{mj})}{(x-s)^2}dx + 4\sum_{l=1}^{\infty}\int_{x_m}^{x_{m+1}}\frac{\prod_{j=0}^{k}(x-x_{mj})}{(x-s+2l\pi)^2}\,dx\\
&\quad + 4\sum_{l=1}^{\infty}\int_{x_m}^{x_{m+1}}\frac{\prod_{j=0}^{k}(x-x_{mj})}{(x-s-2l\pi)^2}\,dx,
\end{aligned} \tag{56}$$

and combining Lemma 4, (28), (55) with (56), we obtain

$$\begin{aligned}
-8h^k\Phi_k(\tau) &= \sum_{i=0}^{n-1}\mathcal{I}_{n,i}^{k}(s)\\
&= \sum_{i=0,i\neq m}^{n-1}\int_{x_i}^{x_{i+1}}\frac{\prod_{j=0}^{k}(x-x_{ij})}{\sin^2\frac{x-s}{2}}dx + \neq\!\!\!\!\!\!\int_{x_m}^{x_{m+1}}\frac{\prod_{j=0}^{k}(x-x_{mj})}{\sin^2\frac{x-s}{2}}dx\\
&= 4\sum_{i=0,i\neq m}^{n-1}\int_{x_i}^{x_{i+1}}\frac{\prod_{j=0}^{k}(x-x_{ij})}{(x-s)^2}dx + 4\,\neq\!\!\!\!\!\!\int_{x_m}^{x_{m+1}}\frac{\prod_{j=0}^{k}(x-x_{mj})}{(x-s)^2}dx\\
&\quad + 4\sum_{i=0}^{n-1}\sum_{l=1}^{\infty}\int_{x_i}^{x_{i+1}}\frac{\prod_{j=0}^{k}(x-x_{ij})}{(x-s+2l\pi)^2}dx + 4\sum_{i=0}^{n-1}\sum_{l=1}^{\infty}\int_{x_i}^{x_{i+1}}\frac{\prod_{j=0}^{k}(x-x_{ij})}{(x-s-2l\pi)^2}dx
\end{aligned}$$

$$= -4\sum_{i=0}^{n-1}\frac{h^k}{2^{k-1}}\psi_k'(2(m-i)+\tau)-4\sum_{i=0}^{n-1}\sum_{l=1}^{\infty}\frac{h^k}{2^{k-1}}\psi_k'(2(m-i-nl)+\tau)$$
$$-4\sum_{i=0}^{n-1}\sum_{l=1}^{\infty}\frac{h^k}{2^{k-1}}\psi_k'(2(m-i+nl)+\tau),$$

i.e.,

$$\begin{aligned}\Phi_k(\tau) &= \frac{1}{2^k}\left[\sum_{i=0}^{n-1}\psi_k'(2(m-i)+\tau)+\sum_{i=0}^{n-1}\sum_{l=1}^{\infty}\psi_k'(2(m-i-nl)+\tau)\right.\\ &\quad\left.+\sum_{i=0}^{n-1}\sum_{l=1}^{\infty}\psi_k'(2(m-i+nl)+\tau)\right]\\ &= \frac{1}{2^k}\left[\sum_{l=-\infty}^{\infty}\sum_{i=0}^{n-1}\psi_k'(2(m-i+nl)+\tau)\right]\\ &= \frac{1}{2^k}\left[\psi_k'(\tau)+\sum_{l=1}^{\infty}\psi_k'(2l+\tau)+\sum_{l=1}^{\infty}\psi_k'(-2l+\tau)\right]\\ &= \frac{1}{2^k}S_k(\tau).\end{aligned}$$

The proof is completed. □

From Theorems 4 and 5, we can easily simplify the proof in [26] for the existence of the zeroes of $\mathcal{S}_k(\tau)$ for any positive integer k.

5 The computation of Cotes coefficients

The Cotes coefficients of Newton–Cotes rules for (3) on the interval can be easily obtained by first expanding $f(x)$ into Taylor series at s and then through some direct calculation. For the finite-part integral (1) on the circle, we have discussed the composite trapezoidal rule in [31] and obtained its Cotes coefficients as a simple form.

From Theorem 2, the convergence rate can be improved by using the higher order Newton–Cotes rules for (1). We can represent Cotes Coefficients as follows:

$$\omega_{ij}^k(s) = \frac{1}{l_{ki}'(x_{ij})}\,⨎_{x_i}^{x_{i+1}}\frac{1}{\sin^2\frac{x-s}{2}}\prod_{m=0,m\neq j}^{k}(x-x_{im})\,dx. \tag{57}$$

Unfortunately, for $k>1$, we cannot get the Cotes coefficients analytically like that for the trapezoidal rule in [31]. A natural question raised is how to compute these coefficients efficiently.

By taking integral by parts for (57), we get

$$\omega_{ij}^{k}(s)=\frac{1}{l_{ki}'(x_{ij})}\left[-2\prod_{\substack{0\le m\le k\\ m\ne j}}(x_{i+1}-x_{im})\cot\frac{x_{i+1}-s}{2}\right.$$
$$\left.+2\prod_{\substack{0\le m\le k\\ m\ne j}}(x_i-x_{im})\cot\frac{x_i-s}{2}+2\int_{x_i}^{x_{i+1}}\sum_{\substack{0\le l\le k\\ l\ne j}}\prod_{\substack{0\le m\le k\\ m\ne l,j}}(x-x_{im})\cot\frac{x-s}{2}\,dx\right],\tag{58}$$

Thus, for computing $\omega_{ij}^{k}(s)$, the main difficulty lies in evaluating the last term of (58). By expanding the polynomial $\sum_{\substack{0\le l\le k\\ l\ne j}}\prod_{\substack{0\le m\le k\\ m\ne l,j}}(x-x_{im})$ at the point s, the problem can be converted as how to evaluate

$$\mathcal{J}_l(x):=\int_0^x t^l\cot\frac{t}{2}\,dt,\quad l=1,2,\ldots,k-1.\tag{59}$$

From [3] and by some modification, the integrals $\mathcal{J}_l(x)$ can be expressed in terms of the values of Clausen functions and zeta functions:

$$\mathcal{J}_l(x)=2\Delta_l+2x^l\log|2\sin\frac{x}{2}|+2l!\sum_{i=1}^{[(l+1)/2]}(-1)^{i-1}\frac{x^{l-2i+1}}{(l-2i+1)!}\mathrm{Cl}_{2i}(x)$$
$$+2l!\sum_{i=1}^{[l/2]}(-1)^{i-1}\frac{x^{l-2i}}{(l-2i)!}\mathrm{Cl}_{2i+1}(x),\quad l=1,2,\ldots,k-1,\tag{60}$$

where

$$\Delta_l=\begin{cases}0, & \text{if } l \text{ is odd},\\ (-1)^{[l/2]}l!\zeta(l+1), & \text{if } l \text{ is even}\end{cases}$$

and

$$\zeta(s)=\sum_{i=1}^{\infty}\frac{1}{i^s}$$

is zeta function. As to the computation of Clausen function $\mathrm{Cl}_n(x)$, we can use the following formulae(which will be discussed in another paper):

$$\mathrm{Cl}_n(x) = (-1)^{[(n+1)/2]}\frac{x^{n-1}}{(n-1)!}\ln\left|2\sin\frac{x}{2}\right| + \frac{(-1)^{[n/2]+1}}{(n-2)!}\sum_{i=0}^{n-2}(-1)^i\binom{n-2}{i}x^i\mathcal{N}_{n-2-i}(x)+\mathcal{P}_n(x), \quad x\in[-\pi,\pi], \tag{61}$$

where $\binom{n}{k}$ is the combination number,

$$\mathcal{P}_n(x) = \sum_{i=2}^{n}(-1)^{[(n-1)/2]+[(i-1)/2]}\frac{x^{n-i}}{(n-i)!}\mathrm{Cl}_i(0), \qquad \mathrm{Cl}_i(0) = \begin{cases} 0, & \text{i even,}\\ \zeta(i), & \text{i odd} \end{cases} \tag{62}$$

and

$$\mathcal{N}_n(x) = \frac{1}{n+1}\left[\frac{x^{n+1}}{n+1} + \sum_{k=1}^{\infty}(-1)^k B_{2k}\frac{x^{2k+n+1}}{(2k+n+1)(2k)!}\right]. \tag{63}$$

Here, B_{2k} denote the Bernoulli numbers. By using the periodicity (12) of Clausen fuctions $\mathrm{Cl}_n(x)$, we can first compute the value of $\mathrm{Cl}_n(x)$ on the interval $[-\pi,\pi]$ by (61), and then extend it to the whole space by periodic extension with period 2π. Thus $\mathcal{J}_l(x)$ can be evaluated by (60). In the actual procdure of computation, since the series in (63) converges exponentially in $[-\pi,\pi]$, we just need to take a few truncation terms N instead of ∞ in (63). The impact of truncation term for errors will be discussed in the next section by numerical experiments.

6 Numerical experiments

In this section, computational results are reported by several examples to confirm our theoretical analysis and to show the efficiency of the algorithms.

Consider the finite-part integral

$$\text{=}\!\!\!\!\!\!\int_{-\pi}^{\pi}\frac{1+3\cos 2x+4\sin 2x}{\sin^2\frac{x-s}{2}}dx, \tag{64}$$

by (1) and a direct calculation, the exact solution is

Table 1 Errors of $\mathcal{Q}_{2n}(f)$

n	$s = x_{[n/4]} + (1+\tau)h/2$			$s = x_n - (1+\tau)h/2$		
	$\tau = 0$	$\tau = \frac{2}{3}$	$\tau = -\frac{1}{3}$	$\tau = 0$	$\tau = \frac{2}{3}$	$\tau = -\frac{1}{3}$
64	0.34973E−3	0.17647E+0	0.12433E+0	0.26854E−3	0.21756E+0	0.14022E+0
128	0.49060E−4	0.47093E−1	0.32191E−1	0.43028E−4	0.52264E−1	0.34165E−1
256	0.64195E−5	0.12122E−1	0.81783E−2	0.60126E−5	0.12770E−1	0.84242E−2
512	0.81885E−6	0.30727E−2	0.20604E−2	0.79248E−6	0.31538E−2	0.20911E−2
1024	0.10334E−6	0.77335E−3	0.51704E−3	0.10168E−6	0.78348E−3	0.52087E−3
Order of convergence	2.931	1.959	1.978	2.845	2.029	2.018

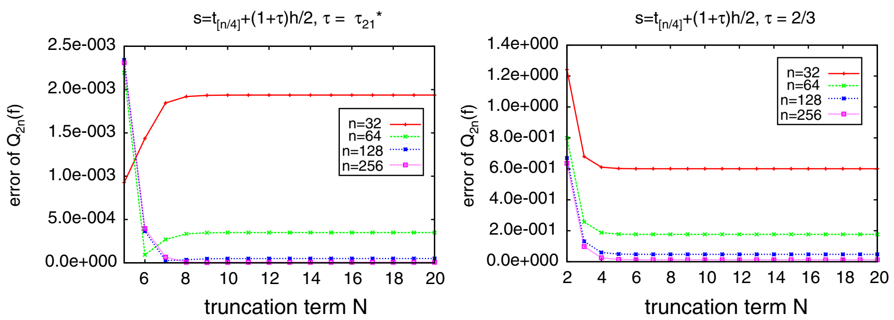

Fig. 1 Truncation error of $\mathcal{Q}_{2n}(f)$

$$\int_{-\pi}^{\pi} \frac{1 + 3\cos 2x + 4\sin 2x}{\sin^2 \frac{x-s}{2}} dx = -8\pi(3\cos 2s + 4\sin 2s), \tag{65}$$

where $s \in (-\pi,\ \pi)$.

Example 1 We use the quadrature rule $\mathcal{Q}_{2n}(f)$ defined by (16) to evaluate (64). Numerical results are presented in the left of Table 1 for a dynamic singular point $s = t_{[n/4]} + (1+\tau)h/2$ and in the right of Table 1 for $s = t_n - (1+\tau)h/2$. The estimated orders of convergence are given in the last row, which are obtained by a least squares fit. In the first case singular point s is not close to the endpoints of the interval $[-\pi, \pi]$ while in the second it approaches the endpoints as h goes to zero. We can see from Table 1 that in both cases errors at the superconvergence points, are $O(h^3)$ which is in good agreement with our theoretical analysis. The effect of the truncation term to the error can be seen in Fig. 1.

Example 2 Here we use $\mathcal{Q}_{3n}(f)$ to evaluate (64). From Table 2, one can see that errors are $O(h^4)$ at the superconvergence points and $O(h^3)$ at the non-superconvergence points, whether the singular point s is close to the endpoints or not, which is in good agreement with our theoretical analysis. The effect of the truncation term to the error can be seen in Fig. 2.

Table 2 Errors of $\mathcal{Q}_{3n}(f)$

n	$s = x_{[n/4]} + (1+\tau)h/2$			$s = x_n - (1+\tau)h/2$		
	$\tau = \tau_{31}^*$	$\tau = \tau_{32}^*$	$\tau = 0$	$\tau = \tau_{31}^*$	$\tau = \tau_{32}^*$	$\tau = 0$
16	0.12369E−1	0.63372E−1	0.15920E+0	0.65470E−2	0.54861E−1	0.45917E−1
32	0.80190E−3	0.40315E−2	0.17656E−1	0.33601E−3	0.34838E−2	0.10254E−1
64	0.50524E−4	0.25302E−3	0.20250E−2	0.18538E−4	0.21852E−3	0.15549E−2
128	0.31623E−5	0.15827E−4	0.24050E−3	0.10786E−5	0.13666E−4	0.21093E−3
256	0.19697E−6	0.98866E−6	0.29238E−4	0.58365E−7	0.84643E−6	0.27378E−4
Order of convergence	3.924	3.965	3.122	4.193	3.996	2.850

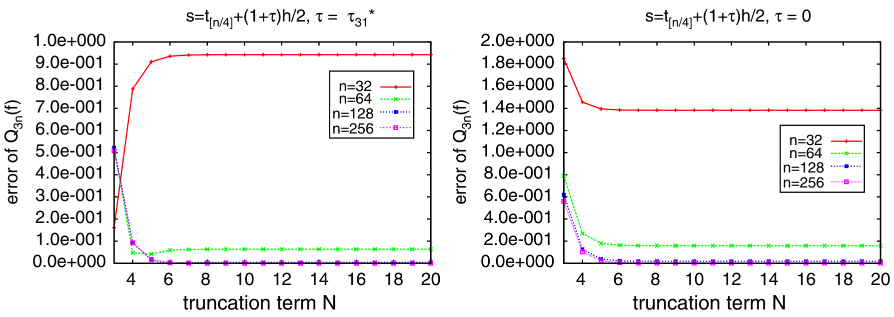

Fig. 2 Truncation error of $\mathcal{Q}_{3n}(f)$

Table 3 Errors of $\mathcal{Q}_{4n}(f)$

n	$s = x_{[n/4]} + (1+\tau)h/2$			$s = x_n - (1+\tau)h/2$		
	$\tau = \tau_{41}^*$	$\tau = \tau_{42}^*$	$\tau = 1/3$	$\tau = \tau_{41}^*$	$\tau = \tau_{42}^*$	$\tau = 1/3$
8	0.54252E−2	0.58413E−2	0.15007E−1	0.77502E−3	0.77813E−2	0.11569E+0
16	0.21323E−3	0.32394E−3	0.37528E−2	0.61500E−4	0.62915E−4	0.70550E−2
32	0.66694E−5	0.97621E−5	0.30559E−3	0.38724E−5	0.26035E−5	0.40889E−3
64	0.18979E−6	0.26417E−6	0.20999E−4	0.14478E−6	0.14464E−6	0.24239E−4
128	0.57391E−8	0.38837E−8	0.13561E−5	0.60325E−8	0.66977E−8	0.14805E−5
Order of convergence	4.963	5.150	3.953	4.741	5.037	4.063

Example 3 Here we use $\mathcal{Q}_{4n}(f)$ to evaluate (64). Numerical results presented in Table 3 show that in all cases errors are $O(h^5)$ at the superconvergence points and $O(h^4)$ at the non-superconvergence points, which is in good agreement with our theoretical analysis. The effect of the truncation term to the error can be seen in Fig. 3.

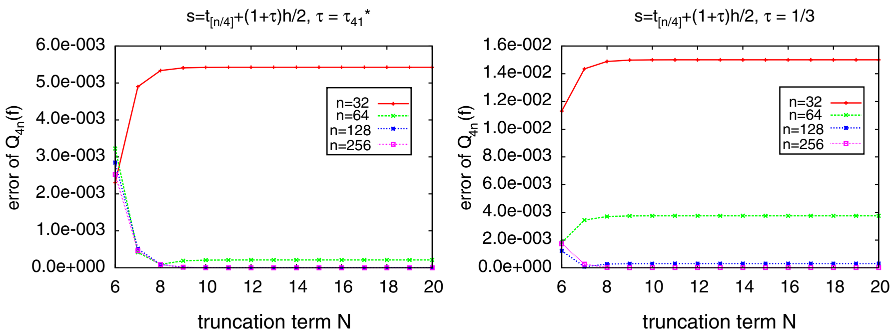

Fig. 3 Truncation error of $Q_{4n}(f)$

7 Concluding remarks

We have proved the superconvergence estimate of the (composite) Newton rules for the finite-part integral (1) and also showed the existence of the superconvergence points. The theoretical results are confirmed by the numerical experiments. Numerical results in the previous section indicate that when the singular point coincides with a superconvergence point, the accuracy can be one order higher than that when the non-superconvergence point is involved. Thus a natural question that can be raised is that whether it is possible to remove the factor $|\ln h|$ from estimate (23). The answer is certainly positive. Actually, we can prove that the superconvergence rate can be $O(h^{k+1})$ provided that $f(x) \in C^{k+2+\alpha}(c; c+2\pi)(0 < \alpha < 1)$. Here we omit this part of the argument just because it involves tedious details similar to the cases discussed in the present paper and its presentation will spoil the structure and make our main idea obscure.

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