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Superconvergence and ultraconvergence of Newton–Cotes rules for supersingular integrals

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ABSTRACT

In this article, the general (composite) Newton–Cotes rules for evaluating Hadamard finite-part integrals with third-order singularity (which is also called "supersingular integrals") are investigated and the emphasis is placed on their pointwise superconvergence and ultraconvergence. The main error of the general Newton–Cotes rules is derived, which is shown to be determined by a certain function $\mathcal{S}'_k(\tau)$. Based on the error expansion, the corresponding modified quadrature rules are also proposed. At last, some numerical experiments are carried out to validate the theoretical analysis.

1. Introduction

How to compute the boundary integrals efficiently arising in boundary element method has been a subject of intensive research in recent years which reduces, sometimes, to the evaluation of integrals of the form

$$\mathcal{I}_p(a,b;s,f) = ⨍_a^b \frac{f(x)}{(x-s)^{p+1}}\mathrm{d}x, \quad s\in(a,b),\ p=1,2,\ldots, \tag{1.1}$$

where $⨍$ denotes an integral in the Hadamard finite-part sense and s the singular point. In general, $\mathcal{I}_p(a,b;s,f)$ is called "hypersingular integral" if $p=1$ and "supersingular integral" if $p\geq 2$.

Integrals (1.1) can be defined in a number of ways and those definitions are mathematically equivalent [1,2]. Here, we adopt the following definition:

$$⨍_a^b \frac{f(x)}{(x-s)^{p+1}}\mathrm{d}x = \lim_{\varepsilon\to 0}\left\{\int_a^{s-\varepsilon}\frac{f(x)}{(x-s)^{p+1}}\mathrm{d}x + \int_{s+\varepsilon}^b \frac{f(x)}{(x-s)^{p+1}}\mathrm{d}x - \frac{2f^{(p-1)}(s)}{\varepsilon}\right\}, \quad s\in(a,b), p=1,2. \tag{1.2}$$

$f(x)$ is said to be finite-part integrable with respect to the weight $(x-s)^{-p-1}$ if the limit on the right hand side of the above equation exists. An sufficient condition for $f(x)$ to be finite-part integrable is that $f^{(p)}(x)$ is Hölder continuous.

Numerous work has been devoted in developing efficient quadrature formulas for hypersingular integrals such as the Gaussian method [3–6], the Newton–Cotes method [7–16], the transformation method [17,18] and some other methods [19,

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20]. The composite Newton–Cotes rule is a commonly used one in many areas due to its ease of implementation and flexibility of mesh. Error analysis of Newton–Cotes rules for Riemann integrals has been well done. The accuracy of Newton–Cotes rules for the Riemann integrals is $O(h^{k+1})$ for odd k and $O(h^{k+2})$ for even k. Due to the high-order singularity of the kernels, the Newton–Cotes rules for Hadamard finite-part integrals (including hypersingular and supersingular integrals) are less accurate than their counterparts for Riemann integrals.

As an efficient method to improve the accuracy of boundary element analysis, Newton–Cotes rules for hypersingular integrals have been intensively studied. The superconvergence phenomenons of trapezoidal rule and Simpson's rule for hypersingular integrals were firstly found in [12,11], respectively. Later, the superconvergence of arbitrary degree Newton–Cotes rules for hypersingular integrals was studied in [13]. Recently, Newton–Cotes rules and the corresponding superconvergence for evaluating hypersingular integrals on a circle were discussed in [21,22].

Integrals with kernels beyond hypersingularity have not been extensively studied, and references [23,7,24–28,12,29,30] may be the entire literature on the subject. The Newton–Cotes rule for such integrals was firstly studied in [7], where the error estimate for Simpson's rule was obtained. Then, the trapezoidal rule was discussed in [12], where this rule was shown to be divergent in general, but exhibit the ultraconvergence phenomenon[1] when the singular point s is located at the middle point of each subinterval away from two endpoints. Recently, Zhang et al. [29] discussed the superconvergence phenomenon of the Simpson's rule.

This article focuses on the superconvergence and ultraconvergence of arbitrary degree Newton–Cotes rules for supersingular integrals. We show that the main error is determined by the function $\mathcal{S}'_k(\tau)$, defined by

$$\mathcal{S}'_k(\tau) := \psi''_k(\tau) + \sum_{i=1}^{\infty} \left[\psi''_k(2i+\tau) + \psi''_k(-2i+\tau)\right], \quad \tau \in (-1, 1), \tag{1.3}$$

where ψ_k is a function of second kind associated with a polynomial of equally distributed zeros. If $\mathcal{S}'_k(\tau) = 0$, i.e., the local coordinate of the singular point s is the zero of $\mathcal{S}'_k(\tau)$, we can easily get the superconvergence rate which is one order higher than the global one. Then, by the error expansion, we propose some modified quadrature rules and obtain their ultraconvergence result at some special points.

The rest of this article is organized as follows. In Section 2, some basic formulas of the general (composite) Newton–Cotes rules and preliminaries are introduced. In Section 3, we present our main result of superconvergence and ultraconvergence, and some modified quadrature rules are proposed. In Section 4, the computation of $\mathcal{S}'_k(\tau)$ is considered. The proof of our main result is given in Section 5. Several numerical examples are provided to validate our analysis in the last section.

2. Preliminaries

Let $a = x_0 < x_1 < \cdots < x_{n-1} < x_n = b$ be a uniform partition of the interval $[a, b]$ with mesh size $h = (b-a)/n$. 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 $[x_i, x_{i+1}]$. Moreover, we define the piecewise Lagrangian polynomial interpolation by

$$\mathcal{F}_{kn}(x) = \sum_{j=0}^{k} f(x_{ij}) \frac{\ell_{ki}(x)}{(x - x_{ij})\ell'_{ki}(x_{ij})}, \quad x \in [x_i, x_{i+1}], \tag{2.1}$$

where

$$\ell_{ki}(x) = \prod_{j=0}^{k} (x - x_{ij}). \tag{2.2}$$

Replacing $f(x)$ in (1.1) with $p = 2$ by $\mathcal{F}_{kn}(x)$ gives the general (composite) Newton–Cotes rule

$$\mathcal{Q}_{kn}(s, f) := \,=\!\!\!\!\!\!\int_a^b \frac{\mathcal{F}_{kn}(x)}{(x-s)^3} \mathrm{d}x = \sum_{i=0}^{n-1} \sum_{j=0}^{k} \omega_{ij}^{(k)} f(x_{ij}) = \mathcal{I}_2(f, s) - \mathcal{E}_{kn}(f), \tag{2.3}$$

[1] For Newton–Cotes rule, the rule is said to exhibit "superconvergence" at $s \in (a, b)$, provided that the convergence rate is one order higher than the global one, and "ultraconvergence" if the convergence rate is two order higher than the global one.

where $\mathcal{E}_{kn}(f)$ denotes the error functional and

$$\omega_{ij}^{(k)} = \frac{1}{\ell'_{ki}(x_{ij})} \int_{x_i}^{x_{i+1}} \frac{1}{(x-s)^3} \prod_{m=0, m\neq j}^{k} (x - x_{im}) \mathrm{d}x. \tag{2.4}$$

In the following, C will denote a generic positive constant which is independent of h and s but which may depend on k and bounds of the derivatives of $f(x)$.

The Simpson's rule for supersingular integral $\mathcal{I}_2(a, b; s, f)$ was studied in [7], where the error estimate was given by

$$|\mathcal{E}_{2n}(f)| \le C\gamma^{-2}(\tau)h, \tag{2.5}$$

where

$$\gamma(\tau) = \min_{0\le i\le n} \frac{|s - x_i|}{h} = \frac{1-|\tau|}{2}, \tag{2.6}$$

and τ is the local coordinate of the singular point s.

We present the error estimate of general (composite) Newton–Cotes rules of arbitrary degree in the following theorem, whose proof can be obtained analogously in [10].

Theorem 2.1. *Assume $f(x) \in C^{k+1}[a, b]$ and $s \neq x_i$ for any $i = 0, 1, 2, \ldots, n$. For the general (composite) Newton–Cotes rule $\mathcal{Q}_{kn}(s, f)$ defined in (2.3), there holds at $s = \hat{x}_i(\tau) \in [x_i, x_{i+1}]$*

$$|\mathcal{E}_{kn}(f)| \le C\gamma^{-1}(\tau)h^{k-1}, \tag{2.7}$$

where $\gamma(\tau)$ is defined in (2.6).

Compared with hypersingular integrals, the global convergence rate of the (composite) Newton–Cotes rule for supersingular integrals ($p = 2$) is one order lower. Especially, we can see from (2.7) that the trapezoidal rule does not converge in general.

Let

$$\phi_k(\tau) = \prod_{j=0}^{k}(\tau - \tau_j) = \prod_{j=0}^{k}\left(\tau - \frac{2j-k}{k}\right) \tag{2.8}$$

and define

$$\psi_k(t) = \begin{cases} -\dfrac{1}{2}\displaystyle{-\!\!\!\!\!\!\int}_{-1}^{1} \frac{\phi_k(\tau)}{\tau - t}\mathrm{d}\tau, & |t| < 1, \\ -\dfrac{1}{2}\displaystyle\int_{-1}^{1} \frac{\phi_k(\tau)}{\tau - t}\mathrm{d}\tau, & |t| > 1. \end{cases} \tag{2.9}$$

It is known that if ϕ_k is the Legendre polynomial, ψ_k defines the Legendre function of the second kind (see e.g., [31,32]). The supersingular integral is related to hypersingular integral and the usual Cauchy principal value integral by

$$\int_a^b \frac{f(x)}{(x-s)^3}\mathrm{d}x = \frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}s}\left(\int_a^b \frac{f(x)}{(x-s)^2}\mathrm{d}x\right) = \frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}s^2}\left({-\!\!\!\!\!\!\int}_a^b \frac{f(x)}{x-s}\mathrm{d}x\right). \tag{2.10}$$

By (2.9) and (2.10), we have

$$\psi'_k(t) = \begin{cases} -\dfrac{1}{2}\displaystyle\int_{-1}^{1} \frac{\phi_k(\tau)}{(\tau - t)^2}\mathrm{d}\tau, & |t| < 1, \\ -\dfrac{1}{2}\displaystyle\int_{-1}^{1} \frac{\phi_k(\tau)}{(\tau - t)^2}\mathrm{d}\tau, & |t| > 1, \end{cases} \tag{2.11}$$

$$\psi''_k(t) = \begin{cases} -\displaystyle\int_{-1}^{1} \frac{\phi_k(\tau)}{(\tau - t)^3}\mathrm{d}\tau, & |t| < 1, \\ -\displaystyle\int_{-1}^{1} \frac{\phi_k(\tau)}{(\tau - t)^3}\mathrm{d}\tau, & |t| > 1. \end{cases} \tag{2.12}$$

Furthermore, we define

$$\varphi_{k+1}(t) = 2\psi'_k(t) + t\psi''_k(t). \tag{2.13}$$

Let $\mathcal{J} := (-\infty, -1) \cup (-1, 1) \cup (1, +\infty)$, define the operator $\mathcal{W} : C(\mathcal{J}) \to C(-1, 1)$ as

$$\mathcal{W}f(\tau) := f(\tau) + \sum_{i=1}^{\infty}[f(2i+\tau) + f(-2i+\tau)], \quad \tau \in (-1, 1). \tag{2.14}$$

Obviously, $\mathcal{W}$ is a linear operator. By (2.14), we can write

$$\mathcal{S}_k(\tau) = \mathcal{W}\psi_k'(\tau), \tag{2.15}$$

$$\mathcal{S}_k'(\tau) = \mathcal{W}\psi_k''(\tau). \tag{2.16}$$

Moreover, we define

$$\tilde{\mathcal{S}}_{k+1}(\tau) = \mathcal{W}\varphi_{k+1}(\tau). \tag{2.17}$$

Let P_l and Q_l denote the Legendre polynomial of degree l and the associated Legendre function of the second kind, respectively.

The proof of the following lemma can be obtained along the line of Lemma 3.1 in [13].

Lemma 2.2. *Let $\psi_k(t)$ and $\varphi_{k+1}(t)$ be defined in (2.9) and (2.13), respectively. Then*

$$\psi_k(t) = \begin{cases} \sum_{i=1}^{k_1+1} \omega_{2i-1} Q_{2i-1}(t), & k = 2k_1, \\ \sum_{i=0}^{k_1} \omega_{2i} Q_{2i}(t), & k = 2k_1 - 1, \end{cases} \tag{2.18}$$

$$\psi_k'(t) = \begin{cases} \sum_{i=1}^{k_1} a_i Q_{2i}(t), & k = 2k_1, \\ \sum_{i=1}^{k_1} b_i Q_{2i-1}(t), & k = 2k_1 - 1, \end{cases} \tag{2.19}$$

$$\psi_k''(t) = \begin{cases} \sum_{i=1}^{k_1} a_i Q_{2i}'(t), & k = 2k_1, \\ \sum_{i=1}^{k_1} b_i Q_{2i-1}'(t), & k = 2k_1 - 1, \end{cases} \tag{2.20}$$

and

$$\varphi_{k+1}(t) = \begin{cases} \sum_{i=1}^{k_1} a_i \left[2Q_{2i}(t) + tQ_{2i}'(t)\right], & k = 2k_1, \\ \sum_{i=1}^{k_1} b_i \left[2Q_{2i-1}(t) + tQ_{2i-1}'(t)\right], & k = 2k_1 - 1, \end{cases} \tag{2.21}$$

where

$$\omega_i = \frac{2i+1}{2} \int_{-1}^{1} \phi_k(\tau) P_i(\tau) \mathrm{d}\tau,$$

and

$$a_i = -(4i+1) \sum_{j=1}^{i} \omega_{2j-1}, \qquad b_i = -(4i-1) \sum_{j=1}^{i} \omega_{2j-2}.$$

3. Main result

Define

$$\mathcal{B}_k(\tau) = 2(k+2)\mathcal{S}_k(\tau) - (k+1)\tilde{\mathcal{S}}_{k+1}(\tau). \tag{3.1}$$

Our main result is given in the following theorem.

Theorem 3.1. *Assume $f(x) \in C^{k+3}[a, b]$ and let $\mathcal{S}_k'(\tau)$ and $\mathcal{B}_k(\tau)$ be defined by (2.16) and (3.1), respectively. Then, for the general (composite) Newton–Cotes rule $\mathcal{Q}_{kn}(s, f)$, there holds at $s = \hat{x}_i(\tau)$*

$$\mathcal{E}_{kn}(f) = -\frac{h^{k-1} f^{(k+1)}(s)}{2^{k-1}(k+1)!} \mathcal{S}_k'(\tau) - \frac{h^k f^{(k+2)}(s)}{2^k (k+2)!} \mathcal{B}_k(\tau) + \mathcal{E}_{kn}^1(f), \tag{3.2}$$

Table 1
Superconvergence points of Newton–Cotes rules.

k	Superconvergence points
1	0
2	±0.6666666666666667
3	0, ±0.7691593399598297
4	±0.3071649777724334, ±0.8827331070858399
5	0, ±0.4803784858889886, ±0.8844060476840933

where

$$|\mathcal{E}^1_{kn}(f)| \le C(\gamma^{-2}(\tau) + \eta(s) + |\ln h|)h^{k+1}, \tag{3.3}$$

with $\gamma(\tau)$ defined in (2.6) and

$$\eta(s) = \max\left\{\frac{1}{(s-a)^2}, \frac{1}{(b-s)^2}\right\}. \tag{3.4}$$

Corollary 3.2. *Under the same assumption of Theorem 3.1, when τ^* is a zero of $\mathcal{S}'_k(\tau)$, there holds $s = \hat{x}_i(\tau^*)$*

$$\mathcal{E}_{kn}(f) = -\frac{h^k f^{(k+2)}(s)}{2^k(k+2)!}\mathcal{B}_k(\tau^*) + \mathcal{E}^2_{kn}(f), \tag{3.5}$$

where

$$|\mathcal{E}^2_{kn}(f)| \le C(\gamma^{-2}(\tau^*) + \eta(s) + |\ln h|)h^{k+1} \tag{3.6}$$

and $\eta(s)$ is defined in (3.4).

Remark 3.3. Actually, Corollary 3.2 shows the superconvergence phenomenon, since the convergence rate of the Newton–Cotes rule $\mathcal{Q}_{kn}(s,f)$ at the superconvergence points $s = \hat{x}_i(\tau^*)$ is improved one order higher than the global one.

Generally speaking, the singular point is probably not a superconvergence point and the accuracy of Newton–Cotes rule $\mathcal{Q}_{kn}(s,f)$ can only be $O(h^{k-1})$. To apply this superconvergence result in practical computation, we may translate the interior mesh points to get a new mesh $a = x'_0 < x'_1 < \cdots < x'_n = b$ in which the singular point is located at a superconvergence point. Obviously, the new mesh is still uniform except two shorter or longer subintervals near the endpoints. It is not difficult to extend the above result to this kind of grid.

We list the local coordinate of superconvergence points, i.e., the zeros of $\mathcal{S}'_k(\tau)$ with 16 digits in Table 1 for different k.

From Theorem 3.1, we suggest a modified quadrature rule $\tilde{\mathcal{Q}}_{kn}(s,f)$, defined by

$$\tilde{\mathcal{Q}}_{kn}(s,f) = \mathcal{Q}_{kn}(s,f) - \frac{h^{k-1}f^{(k+1)}(s)}{2^{k-1}(k+1)!}\mathcal{S}'_k(\tau). \tag{3.7}$$

Theorem 3.4. *Under the same assumption of Theorem 3.1, for the modified Newton–Cotes rule $\tilde{\mathcal{Q}}_{kn}(s,f)$ defined by (3.7), there holds at $s = \hat{x}_i(\tau)$*

$$\mathcal{I}_2(f,s) - \tilde{\mathcal{Q}}_{kn}(s,f) = -\frac{h^k f^{(k+2)}(s)}{2^k(k+2)!}\mathcal{B}_k(\tau) + \mathcal{E}^1_{kn}(f), \tag{3.8}$$

where $\mathcal{E}^1_{kn}(f)$ is bounded in (3.3).

Remark 3.5. The modified composite Newton–Cotes rule $\tilde{\mathcal{Q}}_{kn}(s,f)$ is a quadrature rule with kth-order accuracy, but it should be noted that this rule may be still invalid if the singular point s is too closely to the nodal points due to the factor $\gamma^{-2}(\tau)$ in $\mathcal{E}^1_{kn}(f)$.

Lemma 3.6. *For even k and $\tau = 0$, there holds*

$$\mathcal{B}_k(\tau) = \mathcal{S}_k(\tau) = \tilde{\mathcal{S}}_{k+1}(\tau) = 0. \tag{3.9}$$

Proof. By the classic identity of the Legendre function of second kind,

$$Q_l(-t) = (-1)^{l+1}Q_l(t), \quad |t| \ne 1,\ l = 0, 1, \ldots, \tag{3.10}$$

and from (2.19) we get

$$\psi_k'(-t) = -\psi_k'(t) \tag{3.11}$$

for even k. Thus, we can see from (2.15) that

$$\mathcal{S}_k(-\tau) = -\mathcal{S}_k(\tau), \tag{3.12}$$

which means $\tau = 0$ is a zero of $\mathcal{S}_k(\tau)$ with even k.

From (3.10), we have

$$Q_l'(-t) = (-1)^{l+2} Q_l'(t), \quad |t| \neq 1,\ l = 0, 1, \ldots, \tag{3.13}$$

which leads to

$$\varphi_{k+1}(-t) = -\varphi_{k+1}(t)$$

for even k. By (2.17), we prove $\tau = 0$ is a zero of $\tilde{\mathcal{S}}_{k+1}(\tau)$ with even k. Furthermore, we can easily see from (3.1) that $\tau = 0$ is also a zero of $\mathcal{B}_k(\tau)$ with even k. □

Theorem 3.7. *Under the same assumption of Theorem 3.1, for the modified Newton–Cotes rule $\tilde{\mathcal{Q}}_{kn}(s, f)$ with even k, there holds at $s = \hat{x}_i(0)$,*

$$\left|\mathcal{I}_2(f, s) - \tilde{\mathcal{Q}}_{kn}(s, f)\right| \le C(4 + \eta(s) + |\ln h|)h^{k+1}, \tag{3.14}$$

where $\eta(s)$ is defined in (3.4).

Remark 3.8. From Theorem 3.7, we know that at the midpoint of each subinterval away from the endpoints, the convergence rate of the modified Newton–Cotes rule with even degree k is $O(h^{k+1})$. It is two order higher than that of the original Newton–Cotes rule and this phenomenon is called here as ultraconvergence.

4. Calculation of $\mathcal{S}_k'(\tau)$

In the above section, we have discussed the modified quadrature rule, there arises a problem how we calculate $\mathcal{S}_k'(\tau)$ exactly and quickly. First, we recall some notation in [22]. Define

$$\Phi_k(\tau) = \begin{cases} \displaystyle\sum_{i=1}^{k_1} (-1)^{k_1-i} \frac{(2k_1-2i+2)!}{(2\pi)^{2k_1-2i+1}} \sigma_{2i-1}^{2k_1} \mathrm{Cl}_{2k_1-2i+2}[(1+\tau)\pi], & k = 2k_1; \\ \displaystyle\sum_{i=1}^{k_1} (-1)^{k_1-i} \frac{(2k_1-2i+1)!}{(2\pi)^{2k_1-2i}} \sigma_{2i-1}^{2k_1-1} \mathrm{Cl}_{2k_1-2i+1}[(1+\tau)\pi], & k = 2k_1 - 1, \end{cases} \tag{4.1}$$

where $\mathrm{Cl}_n(x)$ are Clausen functions, defined by

$$\mathrm{Cl}_n(x) = \begin{cases} \displaystyle\sum_{k=1}^{\infty} \frac{\sin(kx)}{k^n}, & n \text{ even}, \\ \displaystyle\sum_{k=1}^{\infty} \frac{\cos(kx)}{k^n}, & n \text{ odd}, \end{cases} \tag{4.2}$$

and

$$\sigma_i^k = \sigma_i\left(\frac{1}{k}, \frac{2}{k}, \ldots, \frac{k}{k}\right) \tag{4.3}$$

with

$$\begin{cases} \sigma_0(x_1, \ldots, x_k) = 1, \\ \sigma_i(x_1, \ldots, x_k) = \displaystyle\sum_{1 \le j_1 < j_2 < \cdots < j_i \le k} x_{j_1} \cdots x_{j_i}, \quad 1 \le i \le k. \end{cases} \tag{4.4}$$

Especially,

$$\mathrm{Cl}_1(x) = -\ln\left|2\sin\frac{x}{2}\right|. \tag{4.5}$$

From (4.5) and the identity in [22]

$$\mathcal{S}_k(\tau) = 2^k \Phi_k(\tau), \tag{4.6}$$

we get the following result.

Theorem 4.1. *Let $\mathcal{S}_k(\tau)$ and $\Phi_k(\tau)$ be defined in (2.15) and (4.6), respectively. Then, we have*

$$\mathcal{S}'_k(\tau) = 2^k \Phi'_k(\tau), \tag{4.7}$$

where

$$\Phi'_k(\tau) = \begin{cases} \sum_{i=1}^{k_1} (-1)^{k_1-i} \frac{(2k_1-2i+2)!}{(2\pi)^{2k_1-2i}} \sigma_{2i-1}^{2k_1} \mathrm{Cl}_{2k_1-2i+1}[(1+\tau)\pi], & k = 2k_1; \\ \sum_{i=1}^{k_1-1} \frac{(-1)^{k_1-i}(2k_1-2i+1)!}{(2\pi)^{2k_1-2i}} \sigma_{2i-1}^{2k_1-1} \mathrm{Cl}_{2k_1-2i}[(1+\tau)\pi] + \frac{\pi}{2}\sigma_{2k_1-1}^{2k_1-1} \tan\left(\frac{\tau\pi}{2}\right), & k = 2k_1 - 1. \end{cases} \tag{4.8}$$

Now, we mainly give some remarks about trapezoidal rule and Simpson's rule for evaluating the supersingular integral $\mathcal{I}_2(a, b; f, s)$, which have been discussed in [12,29], respectively.

Case 1. Trapezoidal rule ($k = 1$).

We can see that from Corollary 3.2 the superconvergence rate of trapezoidal rule should be $O(h)$, but in fact this rule can achieve its ultraconvergence rate $O(h^2)$, which has been stated in [12]. Now, we explain why this ultraconvergence phenomenon appears in a simple way. By Theorem 4.1 and straightforward calculation, we get

$$\mathcal{S}'_1(\tau) = 2\Phi'_1(\tau) = \pi \tan\left(\frac{\tau\pi}{2}\right), \tag{4.9}$$

$$\begin{aligned} \mathcal{S}_1(\tau) &= 2\Phi_1(\tau) = -2\ln\left[2\cos\left(\frac{\tau\pi}{2}\right)\right], \\ \tilde{\mathcal{S}}_2(\tau) &= \mathcal{S}'_2(\tau) = -4\Phi'_2(\tau) = -6\ln\left[2\cos\left(\frac{\tau\pi}{2}\right)\right] \end{aligned} \tag{4.10}$$

which leads to

$$\mathcal{B}_1(\tau) = 6\mathcal{S}_1(\tau) - 2\tilde{\mathcal{S}}_2(\tau) = 0,$$

i.e., for any τ the second term in (3.2) vanishes. Furthermore, if $\tau = 0$, from (4.9) we see that the first term in (3.2) also disappears, and thus the accuracy of $O(h^2)$ can be obtained.

Obviously, the modified trapezoidal rule

$$\tilde{\mathcal{Q}}_{1n}(s, f) = \mathcal{Q}_{1n}(s, f) - \frac{\pi}{2} f''(s) \tan\left(\frac{\tau\pi}{2}\right) \tag{4.11}$$

is also an quadrature method with accuracy $O(h^2)$.

Case 2. Simpson's rule ($k = 2$).

By Theorem 4.1, we see that

$$\mathcal{S}'_2(\tau) = -4\Phi'_2(\tau) = -6\ln\left[2\cos\left(\frac{\tau\pi}{2}\right)\right]. \tag{4.12}$$

From Theorem 3.7, we see that the modified Simpson's rule

$$\tilde{\mathcal{Q}}_{2n}(s, f) = \mathcal{Q}_{2n}(s, f) + \frac{h}{2} f'''(s) \ln\left[2\cos\left(\frac{\tau\pi}{2}\right)\right] \tag{4.13}$$

has an ultraconvergence rate $O(h^3)$ at $\tau = 0$.

Case 3. $k > 2$.

For $k > 2$, we present $\mathcal{S}'_k(\tau)$ as the combination of some Clausen functions, and thus the key is the evaluation of Clausen function. Here, we adopt a fast algorithm to compute $\mathrm{Cl}_n(x)$, which has the form

$$\begin{aligned} \mathrm{Cl}_n(x) \; &= \; (-1)^{[(n+1)/2]} \frac{x^{n-1}}{(n-1)!} \ln\left|2\sin\frac{x}{2}\right| \\ &+ \frac{(-1)^{[n/2]+1}}{(n-2)!} \sum_{i=0}^{n-2} (-1)^i \binom{n-2}{i} x^i \mathcal{N}_{n-2-i}(x) + \mathcal{P}_n(x), \quad x \in [-\pi, \pi]. \end{aligned} \tag{4.14}$$

Here, $\binom{n}{k}$ is the binomial coefficient,

$$\mathcal{P}_n(x) = \sum_{i=2}^{n} (-1)^{[(n-1)/2]+[(i-1)/2]} \frac{x^{n-i}}{(n-i)!} \mathrm{Cl}_i(0) \tag{4.15}$$

with

$$\mathrm{Cl}_i(0) = \begin{cases} 0, & i \text{ even}, \\ \zeta(i), & i \text{ odd}, \end{cases}$$

where $\zeta(s) = \sum_{i=1}^{\infty} \frac{1}{i^s}$ is the zeta function,

$$\mathcal{N}_n(x) = \frac{1}{n+1} \left[\frac{x^{n+1}}{n+1} + \sum_{k=1}^{\infty} (-1)^k B_{2k} \frac{x^{2k+n+1}}{(2k+n+1)(2k)!} \right], \tag{4.16}$$

and B_k denotes the Bernoulli number. In fact, the series in (4.14) converge exponentially in $[-\pi, \pi]$, and we just need to retain a few terms instead of infinite terms in the practical computation.

5. Proof of Theorem 3.1

In this section, we complete the proof of Theorem 3.1. Let

$$D_i^k(x) = (k+2)(x-s) - (k+1)(x - \hat{x}_i(0)), \tag{5.1}$$

where $\hat{x}_i(0) = \sum_{j=0}^{k} x_{ij}/(k+1)$.

Lemma 5.1. *Let $f(x) \in C^{k+3}[a, b]$ and $\mathcal{F}_{kn}(x)$ be defined in (2.1), then for $x \in [x_i, x_{i+1}]$ and $s \in (a, b)$, there holds*

$$f(x) - \mathcal{F}_{kn}(x) = \frac{f^{(k+1)}(s)}{(k+1)!} \ell_{ki}(x) + \frac{f^{(k+2)}(s)}{(k+2)!} D_i^k(x) \ell_{ki}(x) + \mathcal{H}_{ki}(x), \tag{5.2}$$

where $D_i^k(x)$ is defined in (5.1) and

$$\mathcal{H}_{ki}(x) = \mathcal{H}_{ki}^1(x) + \mathcal{H}_{ki}^2(x) + \mathcal{H}_{ki}^3(x) \tag{5.3}$$

with

$$\begin{aligned} \mathcal{H}_{ki}^1(x) &= \sum_{j=0}^{k} \frac{f^{(k+3)}(\theta_{ij})}{(k+3)!\ell_{ki}'(x_{ij})} (x_{ij} - x)^{k+2} \ell_{ki}(x), \\ \mathcal{H}_{ki}^2(x) &= \frac{f^{(k+3)}(\eta_i)}{2(k+1)!} (x-s)^2 \ell_{ki}(x), \\ \mathcal{H}_{ki}^3(x) &= -\frac{(k+1) f^{(k+3)}(\xi_i)}{(k+2)!} (x-s)(x - \hat{x}_i(0)) \ell_{ki}(x) \end{aligned} \tag{5.4}$$

and $\theta_{ij}, \eta_i, \xi_i \in (x_i, x_{i+1})$. Moreover, there holds for $x \in [x_i, x_{i+1}]$

$$|\mathcal{H}_{ki}^1(x)| \le Ch^{k+3}. \tag{5.5}$$

Proof. Taking Taylor expansion for $f(x_{ij})$ at x, we have

$$f(x) - \mathcal{F}_{kn}(x) = \frac{f^{(k+1)}(x)}{(k+1)!} \ell_{ki}(x) - \frac{(k+1) f^{(k+2)}(x)}{(k+2)!} \left[x - \hat{x}_i(0) \right] \ell_{ki}(x) + \sum_{j=0}^{k} \frac{f^{(k+3)}(\theta_{ij})}{(k+3)!\ell_{ki}'(x_{ij})} (x_{ij} - x)^{k+2} \ell_{ki}(x), \tag{5.6}$$

where we have used

$$\sum_{j=0}^{k} \frac{(x_{ij} - x)^q}{\ell_{ki}'(x_{ij})} = \begin{cases} 0, & q < k, \\ 1, & q = k, \\ (k+1)(\hat{x}_i(0) - x), & q = k+1. \end{cases} \tag{5.7}$$

Applying Taylor expansion to $f^{(k+1)}(x)$ and $f^{(k+2)}(x)$ in (5.6) at s, we have

$$\begin{aligned} f^{(k+1)}(x) &= f^{(k+1)}(s) + f^{(k+2)}(s)(x-s) + \frac{f^{(k+3)}(\eta_i)}{2} (x-s)^2, \\ f^{(k+2)}(x) &= f^{(k+2)}(s) + f^{(k+3)}(\xi_i)(x-s). \end{aligned} \tag{5.8}$$

Therefore, (5.2) can be obtained directly from (5.6) and (5.8), and (5.5) is followed by the definition of $\mathcal{H}_{ki}^1(x)$. □

Lemma 5.2. *Let $\psi_k(x)$ and $\eta(s)$ be defined by (2.9) and (3.4), respectively, then we have*

$$\left|\sum_{i=m+1}^{\infty}\psi_k'(2i+\tau)+\sum_{i=n-m}^{\infty}\psi_k'(-2i+\tau)\right|\le C\sqrt{\eta(s)}h, \tag{5.9}$$

$$\left|\sum_{i=m+1}^{\infty}\psi_k''(2i+\tau)+\sum_{i=n-m}^{\infty}\psi_k''(-2i+\tau)\right|\le C\eta(s)h^2, \tag{5.10}$$

$$\left|\sum_{i=m+1}^{\infty}\varphi_{k+1}(2i+\tau)+\sum_{i=n-m}^{\infty}\varphi_{k+1}(-2i+\tau)\right|\le C\eta(s)h^2. \tag{5.11}$$

Proof. Let $C_1=\max_{-1\le\tau\le1}|\phi_k(\tau)|$, from (2.11)–(2.13), we have

$$\begin{aligned}
|\psi_k'(t)|&\le\frac{C_1}{2}\int_{-1}^{1}\frac{d\tau}{|\tau-t|^2},\\
|\psi_k''(t)|&\le C_1\int_{-1}^{1}\frac{d\tau}{|\tau-t|^3},\\
|\varphi_k(t)|&\le C_1\int_{-1}^{1}\frac{d\tau}{|\tau-t|^3}.
\end{aligned}\tag{5.12}$$

Noting that $s=x_m+\frac{\tau+1}{2}h=a+(m+\frac{\tau+1}{2})h$, we have $2(s-a)/h=\tau+2m+1$ and

$$\begin{aligned}
\left|\sum_{i=m+1}^{\infty}\psi_k'(2i+\tau)\right|&\le\frac{C_1}{2}\sum_{i=m+1}^{\infty}\int_{-1}^{1}\frac{dt}{|2i+\tau-t|^2}\\
&=\frac{C_1}{2}\int_{\tau+2m+1}^{\infty}\frac{dx}{x^2}=\frac{C_1}{2(\tau+2m+1)}=\frac{C_1h}{4(s-a)}.
\end{aligned}\tag{5.13}$$

On the other hand, since $b=a+nh$, we have $2(b-s)/h=2(n-m)-1-\tau$ and

$$\begin{aligned}
\left|\sum_{i=n-m}^{\infty}\psi_k'(\tau-2i)\right|&\le\frac{C_1}{2}\sum_{i=n-m}^{\infty}\int_{-1}^{1}\frac{dt}{|2i-\tau+t|^2}\\
&=\frac{C_1}{2}\int_{2(n-m)-1-\tau}^{\infty}\frac{dx}{x^2}=\frac{C_1}{2[2(n-m)-1-\tau]}=\frac{C_1h}{4(b-s)}.
\end{aligned}\tag{5.14}$$

Combining (5.13) and (5.14), we get (5.9). Then (5.10) and (5.11) can be obtained in an analogous way. □

Lemma 5.3. *Assume $s\in(x_m,x_{m+1})$ for some m and let $c_i=2(s-x_i)/h-1$, $0\le i\le n-1$. Then, we have*

$$\psi_k'(c_i)=\begin{cases}-\dfrac{2^{k-1}}{h^k}\displaystyle\neq\!\!\!\!\!\!\int_{x_i}^{x_{i+1}}\frac{\ell_{ki}(x)}{(x-s)^2}dx, & i=m,\\[2ex] -\dfrac{2^{k-1}}{h^k}\displaystyle\int_{x_i}^{x_{i+1}}\frac{\ell_{ki}(x)}{(x-s)^2}dx, & i\ne m,\end{cases}\tag{5.15}$$

$$\psi_k''(c_i)=\begin{cases}-\dfrac{2^{k-1}}{h^{k-1}}\displaystyle\neq\!\!\!\!\!\!\int_{x_i}^{x_{i+1}}\frac{\ell_{ki}(x)}{(x-s)^3}dx, & i=m,\\[2ex] -\dfrac{2^{k-1}}{h^{k-1}}\displaystyle\int_{x_i}^{x_{i+1}}\frac{\ell_{ki}(x)}{(x-s)^3}dx, & i\ne m,\end{cases}\tag{5.16}$$

and

$$\varphi_{k+1}(c_i)=2\psi_k'(c_i)+c_i\psi_k''(c_i).\tag{5.17}$$

Proof. (5.15) has been proved in [13]. For (5.16) with $i=m$, we have

$$\psi_k''(c_i)=\frac{d}{dc_i}\psi'(c_i)=\frac{d}{ds}\psi_k'(c_i)\frac{ds}{dc_i}=-\frac{2^{k-1}}{h^{k-1}}\neq\!\!\!\!\!\!\int_{x_i}^{x_{i+1}}\frac{\ell_{ki}(x)}{(x-s)^3}dx.$$

The second identity of (5.16) can be similarly obtained. Finally, (5.17) is a natural consequence of (2.13). □

Lemma 5.4. *Under the same assumptions of Theorem 3.1, for $\mathcal{H}_{km}(x)$ in (5.2), there holds that*

$$\left|⨍_{x_m}^{x_{m+1}} \frac{\mathcal{H}_{km}(x)}{(x-s)^3}\mathrm{d}x\right| \le C\gamma^{-2}(\tau)h^{k+1} \tag{5.18}$$

where $\gamma(\tau)$ is defined in (2.6).

Proof. By the definition of $\mathcal{H}_{km}(x)$, we have

$$|\mathcal{H}_{km}^{(l)}(x)| \le Ch^{k+3-l}, \quad l = 0, 1, 2. \tag{5.19}$$

From the identity

$$⨍_a^b \frac{f(x)}{(x-s)^3}\mathrm{d}x = \frac{f(s)}{2}\left[\frac{1}{(a-s)^2} - \frac{1}{(b-s)^2}\right] - \frac{(b-a)f'(s)}{(b-s)(s-a)} + \frac{f''(s)}{2}\ln\frac{b-s}{s-a} + \int_a^b \frac{f(x)-f(s)-f'(s)(x-s)-f''(s)(x-s)^2/2}{(x-s)^3}\mathrm{d}x, \tag{5.20}$$

we have

$$⨍_{x_m}^{x_{m+1}} \frac{\mathcal{H}_{km}(x)}{(x-s)^3}\mathrm{d}x = \frac{\mathcal{H}_{km}(s)}{2}\left[\frac{1}{(x_m-s)^2} - \frac{1}{(x_{m+1}-s)^2}\right] - \frac{h\mathcal{H}'_{km}(s)}{(x_{m+1}-s)(s-x_m)} + \frac{\mathcal{H}''_{km}(s)}{2}\ln\frac{x_{m+1}-s}{s-x_m} + \int_{x_m}^{x_{m+1}} \frac{\mathcal{H}'''_{km}(\theta(x))}{6}\mathrm{d}x \tag{5.21}$$

where $\theta(x) \in (x_m, x_{m+1})$. Since

$$\left|\frac{\mathcal{H}_{km}(s)}{2}\left[\frac{1}{(x_m-s)^2} - \frac{1}{(x_{m+1}-s)^2}\right]\right| \le C\gamma^{-2}(\tau)h^{k+1}, \tag{5.22}$$

$$\left|\frac{h\mathcal{H}'_{km}(s)}{(x_{m+1}-s)(s-x_m)}\right| \le C\gamma^{-1}(\tau)h^{k+1}, \tag{5.23}$$

$$\left|\frac{\mathcal{H}''_{km}(s)}{2}\ln\frac{x_{m+1}-s}{s-x_m}\right| \le C|\ln\gamma(\tau)|h^{k+1} \tag{5.24}$$

and

$$\left|\int_{x_m}^{x_{m+1}} \frac{\mathcal{H}'''_{km}(\theta(x))}{6}\mathrm{d}x\right| \le Ch^{k+1}, \tag{5.25}$$

(5.18) can be obtained by putting together from (5.21) to (5.25). □

Now, we conclude the proof of Theorem 3.1 by the above lemmas.

Proof of Theorem 3.1. By noting the definitions of $\mathcal{S}'_k(\tau)$ and $\mathcal{B}_k(\tau)$, Lemmas 5.1 and 5.3, we have

$$⨍_a^b \frac{f(x)-\mathcal{F}_{kn}(x)}{(x-s)^3}\mathrm{d}x = \sum_{i=0}^{n-1} ⨍_{x_i}^{x_{i+1}} \frac{f(x)-\mathcal{F}_{kn}(x)}{(x-s)^3}\mathrm{d}x = -\frac{h^{k-1}f^{(k+1)}(s)}{2^{k-1}(k+1)!}\mathcal{S}'_k(\tau) - \frac{h^k f^{(k+2)}(s)}{2^k(k+2)!}\mathcal{B}_k(\tau) + \mathcal{E}_{kn}^1(f), \tag{5.26}$$

where

$$\mathcal{E}_{kn}^1(f) = \mathcal{R}^1(s) + \mathcal{R}^2(s) + \mathcal{R}^3(s) \tag{5.27}$$

and

$$\mathcal{R}^1(s) = ⨍_{x_m}^{x_{m+1}} \frac{\mathcal{H}_{km}(x)}{(x-s)^3}\mathrm{d}x, \tag{5.28}$$

$$\mathcal{R}^2(s) = \sum_{i=0,i\ne m}^{n-1} \int_{x_i}^{x_{i+1}} \frac{\mathcal{H}_{ki}^1(x)}{(x-s)^3}\mathrm{d}x + \sum_{i=0,i\ne m}^{n-1} \int_{x_i}^{x_{i+1}} \frac{\mathcal{H}_{ki}^2(x)}{(x-s)^3}\mathrm{d}x + \sum_{i=0,i\ne m}^{n-1} \int_{x_i}^{x_{i+1}} \frac{\mathcal{H}_{ki}^3(x)}{(x-s)^3}\mathrm{d}x \tag{5.29}$$

and

$$\begin{aligned}\mathcal{R}^3(s) &= \frac{f^{(k+1)}(s)h^{k-1}}{2^{k-1}(k+1)!}\left[\sum_{i=m+1}^{\infty}\psi_k''(2i+\tau)+\sum_{i=n-m}^{\infty}\psi_k''(-2i+\tau)\right]\\ &\quad+\frac{f^{(k+2)}(s)h^k}{2^{k-1}(k+1)!}\left[\sum_{i=m+1}^{\infty}\psi_k'(2i+\tau)+\sum_{i=n-m}^{\infty}\psi_k'(-2i+\tau)\right]\\ &\quad-\frac{f^{(k+2)}(s)(k+1)h^k}{2^k(k+2)!}\left[\sum_{i=m+1}^{\infty}\varphi_{k+1}(2i+\tau)+\sum_{i=n-m}^{\infty}\varphi_{k+1}(-2i+\tau)\right].\end{aligned}\tag{5.30}$$

Now, we estimate these three terms one by one. $\mathcal{R}^1(s)$ can be bounded directly by Lemma 5.4. For the first part of $\mathcal{R}^2(s)$, by (5.5),

$$\left|\sum_{i=0,i\neq m}^{n-1}\int_{x_i}^{x_{i+1}}\frac{\mathcal{H}_{ki}^1(x)}{(x-s)^3}\mathrm{d}x\right|\le Ch^{k+3}\sum_{i=0,i\neq m}^{n-1}\int_{x_i}^{x_{i+1}}\frac{1}{|x-s|^3}\mathrm{d}x\le C\gamma^{-2}(\tau)h^{k+1}.\tag{5.31}$$

For the second part of $\mathcal{R}^2(s)$, by the definition of $\mathcal{H}_{ki}^2(x)$, we get

$$\begin{aligned}\left|\sum_{i=0,i\neq m}^{n-1}\int_{x_i}^{x_{i+1}}\frac{\mathcal{H}_{ki}^2(x)}{(x-s)^3}\mathrm{d}x\right| &= \frac{1}{2(k+1)!}\left|\sum_{i=0,i\neq m}^{n-1}\int_{x_i}^{x_{i+1}}\frac{f^{(k+3)}(\eta_i)\ell_{ki}(x)}{x-s}\mathrm{d}x\right|\\ &\le Ch^{k+1}\sum_{i=0,i\neq m}^{n-1}\int_{x_i}^{x_{i+1}}\frac{1}{|x-s|}\mathrm{d}x\\ &\le C(|\ln h|+|\ln\gamma(\tau)|)h^{k+1}\end{aligned}\tag{5.32}$$

and as to the third part of $\mathcal{R}^2(s)$, by the definition of $\mathcal{H}_{ki}^3(x)$, we get

$$\begin{aligned}\left|\sum_{i=0,i\neq m}^{n-1}\int_{x_i}^{x_{i+1}}\frac{\mathcal{H}_{ki}^3(x)}{(x-s)^3}\mathrm{d}x\right| &= \frac{k+1}{(k+2)!}\left|\sum_{i=0,i\neq m}^{n-1}\int_{x_i}^{x_{i+1}}\frac{f^{(k+3)}(\xi_{ij})(x-\hat{x}_i(0))\ell_{ki}(x)}{(x-s)^2}\mathrm{d}x\right|\\ &\le Ch^{k+2}\sum_{i=0,i\neq m}^{n-1}\int_{x_i}^{x_{i+1}}\frac{1}{(x-s)^2}\mathrm{d}x\\ &\le C\gamma^{-1}(\tau)h^{k+1}.\end{aligned}\tag{5.33}$$

Putting (5.29) and (5.31)–(5.33) together yields

$$|\mathcal{R}^2(s)|\le C(\gamma^{-2}(\tau)+|\ln h|)h^{k+1}.\tag{5.34}$$

As for $\mathcal{R}^3(s)$, by Lemma 5.2, we get

$$|\mathcal{R}^3(s)|\le C\eta(s)h^{k+1}.\tag{5.35}$$

Therefore, (3.3) can be obtained by the above estimates. The proof is completed. □

6. Numerical example

In this section, computational results are reported to confirm our analysis. We adopt a uniform mesh and examine the accuracy of Newton–Cotes rules $\mathcal{Q}_{kn}(k=1,2,3,4)$ and modified Newton–Cotes rules $\tilde{\mathcal{Q}}_{kn}(k=1,2,3,4)$ for dynamic singular points $s=x_{[n/4]}+(1+\tau)h/2$.

Example 6.1. Consider the supersingular integral

$$⨍_0^1\frac{x^3}{(x-s)^3}\mathrm{d}x=1+\frac{s}{2}-\frac{s^3-6s^2-6s}{2(s-1)^2}+3s\ln\frac{1-s}{s},\quad s\in(0,1).\tag{6.1}$$

The left half of Table 2 shows that the accuracy of trapezoidal rule $\mathcal{Q}_{1n}$ at the superconvergence points $\tau=0$ is $O(h^2)$, while the rule does not converge in general. As for the right half of Table 2, the accuracy of modified trapezoidal rule $\tilde{\mathcal{Q}}_{1n}$ are always $O(h^2)$, which coincide with the result in Case 1.

Table 2
Errors of the (modified) trapezoidal rule $\mathcal{Q}_{1n}(s, x^3)$ and $\tilde{\mathcal{Q}}_{1n}(s, x^3)$ with $s = x_{[n/4]} + (1+\tau)h/2$.

n	$\mathcal{Q}_{1n}(s, x^3)$			$\tilde{\mathcal{Q}}_{1n}(s, x^3)$	
	$\tau = 0$	$\tau = -2/3$	$\tau = 2/3$	$\tau = -2/3$	$\tau = 2/3$
256	0.27058E−04	0.40917E+01	0.41342E+01	0.27104E−04	0.27012E−04
512	0.67729E−05	0.40864E+01	0.41076E+01	0.67788E−05	0.67672E−05
1024	0.16943E−05	0.40837E+01	0.40943E+01	0.16951E−05	0.16936E−05
2048	0.42371E−06	0.40824E+01	0.40877E+01	0.42388E−06	0.42355E−06
4096	0.10599E−06	0.40817E+01	0.40844E+01	0.10496E−06	0.10720E−06
Ratio	$h^{1.999}$	–	–	$h^{2.000}$	$h^{1.999}$

Table 3
Errors of the (modified) Simpson's rule $\mathcal{Q}_{2n}(s, x^5+1)$ and $\tilde{\mathcal{Q}}_{2n}(s, x^5+1)$ with $s = x_{[n/4]} + (1+\tau)h/2$.

n	$\mathcal{Q}_{2n}(s, x^5+1)$			$\tilde{\mathcal{Q}}_{2n}(s, x^5+1)$	
	$\tau = 2/3$	$\tau = -2/3$	$\tau = 0$	$\tau = 0$	$\tau = 1/2$
16	0.12780E−01	0.10759E−01	0.10309E+00	0.29008E−03	0.37839E−02
32	0.29060E−02	0.26521E−02	0.45886E−01	0.36893E−04	0.84402E−03
64	0.69023E−03	0.65841E−03	0.21601E−01	0.46503E−05	0.19814E−03
128	0.16802E−03	0.16403E−03	0.10474E−01	0.58370E−06	0.47918E−04
256	0.41436E−04	0.40938E−04	0.51565E−02	0.73146E−07	0.11777E−04
Ratio	$h^{2.067}$	$h^{2.009}$	$h^{1.081}$	$h^{2.988}$	$h^{2.082}$

Table 4
Errors of the modified Simpson's 3/8 rule $\mathcal{Q}_{3n}(s, x^6)$ and $\tilde{\mathcal{Q}}_{3n}(s, x^6)$ with $s = x_{[n/4]} + (1+\tau)h/2$.

n	$\mathcal{Q}_{3n}(s, x^6)$			$\tilde{\mathcal{Q}}_{3n}(s, x^6)$	
	$\tau = \tau_{31}^*$	$\tau = \tau_{32}^*$	$\tau = 1/2$	$\tau = 1/2$	$\tau = 1/3$
8	0.12227E−02	0.30795E−02	0.24453E−01	0.46610E−02	0.30789E−02
16	0.13899E−03	0.31551E−03	0.49177E−02	0.51104E−03	0.34251E−03
32	0.16484E−04	0.35052E−04	0.10920E−02	0.59367E−04	0.40138E−04
64	0.20040E−05	0.41061E−05	0.25656E−03	0.71377E−05	0.48501E−05
128	0.24689E−06	0.49594E−06	0.62130E−04	0.87453E−06	0.59611E−06
Ratio	$h^{3.070}$	$h^{3.150}$	$h^{2.155}$	$h^{3.079}$	$h^{3.069}$

Example 6.2. Consider the supersingular integral

$$\oint_0^1 \frac{x^5+1}{(x-s)^3}\mathrm{d}x = 10s^2 + 5s + \frac{10}{3} + \frac{5s+4}{2s^2} + \frac{s-3}{2s^2(s-1)^2} + 10s^3 \ln\frac{1-s}{s}, \quad s \in (0,1). \tag{6.2}$$

From the left half of Table 3, we know the accuracy of Simpson's rule $\mathcal{Q}_{2n}$ is $O(h^2)$ at the superconvergence points $\tau = \pm 2/3$ and $O(h)$ at the non-superconvergence point. The right half of Table 3 shows that the accuracy of modified Simpson's rule $\tilde{\mathcal{Q}}_{2n}$ can achieve $O(h^3)$ at the point $\tau = 0$, one order higher than those at other points, which confirms our theoretical result in Case 2.

Example 6.3. Consider the supersingular integral

$$\oint_0^1 \frac{x^6}{(x-s)^3}\mathrm{d}x = \frac{60s^5 - 90s^4 + 20s^3 + 5s^2 + 2s + 1}{4(s-1)^2} + 15s^4 \log\frac{1-s}{s}, \quad s \in (0,1). \tag{6.3}$$

The left half of Table 4 shows that the accuracy of $\mathcal{Q}_{3n}$ at the superconvergence points $\tau = \tau_{31}^*, \tau_{32}^*$ is $O(h^3)$, which agrees quite well with the estimate in Corollary 3.2. Here, $\tau = 1/2$ is not a superconvergence point, and one can see that the accuracy at the non-superconvergence point is only $O(h^2)$. The right half of Table 4 shows that the accuracy of $\tilde{\mathcal{Q}}_{3n}$ can achieve $O(h^3)$ in general, which confirms our theoretical result in Theorem 3.7.

Example 6.4. We still consider the supersingular integral (6.3). The left half of Table 5 shows that the accuracy of $\mathcal{Q}_{4n}$ at the superconvergence points $\tau = \tau_{41}^*, \tau_{42}^*$ is $O(h^4)$, while it is only $O(h^3)$ at the non-superconvergence point. The right half of Table 5 shows that the accuracy of $\tilde{\mathcal{Q}}_{4n}$ can achieve $O(h^4)$ at any points and can achieve $O(h^5)$ at the point $\tau = 0$, which confirms our theoretical result in Theorem 3.7.

Table 5
Errors of the (modified) Cotes rule $\mathcal{Q}_{4n}(s, x^6)$ and $\tilde{\mathcal{Q}}_{4n}(s, x^6)$ with $s = x_{[n/4]} + (1+\tau)h/2$.

n	$\mathcal{Q}_{4n}(s, x^6)$			$\tilde{\mathcal{Q}}_{4n}(s, x^6)$	
	$\tau = \tau_{41}^*$	$\tau = \tau_{42}^*$	$\tau = 0$	$\tau = 0$	$\tau = 1/3$
2	0.20611E−02	0.85982E−01	0.53538E−01	0.30010E−03	0.42423E−02
4	0.13543E−03	0.53822E−02	0.10096E−01	0.92391E−06	0.26987E−03
8	0.83906E−05	0.33661E−03	0.10515E−02	0.50810E−08	0.16732E−04
16	0.52890E−06	0.21039E−04	0.11830E−03	0.25259E−09	0.10432E−05
32	0.33564E−07	0.13152E−05	0.13965E−04	0.19391E−10	0.64993E−07
Ratio	$h^{4.099}$	$h^{4.000}$	$h^{3.135}$	$h^{5.180}$	$h^{4.194}$

Table 6
Comparison between Newton–Cotes rule ($k = 2$) and Gaussian method.

n	$\mathcal{F}_1(x)$		$\mathcal{F}_0(x)$	
	NC rule	Gaussian method	NC rule	Gaussian method
6	0.12460	0.84207	0.76574	0.41388E−03
12	0.87935E−01	0.60669	0.27112	0.15390E−03
24	0.62184E−01	0.43325	0.95854E−01	0.55960E−04
48	0.43971E−01	0.30791	0.33889E−01	0.20080E−04
96	0.31092E−01	0.21829	0.11982E−01	0.71535E−05
$n^{-\alpha}$	0.500	0.487	1.500	1.464

Assume $x_{ni}(1 \le i \le n)$ are the zeros of the Legendre polynomial $P_n(x)$, then Gaussian method $\mathcal{G}_n(s, f)$ for evaluating the supersingular integral $I_2(-1, 1; s, f)$ can be derived along the line in [6],

$$\begin{aligned}\mathcal{G}_n(s, f) = &-\frac{2}{n}\sum_{i=1}^{n}\frac{(1-x_{ni})^2[Q_n(x_{ni}) - Q_n(s)]}{P_{n-1}(x_{ni}-s)^3}f(x_{ni})\\ &- 2n\frac{\{(1-s^2)P_n(s)f'(s) - n[P_{n-1}(s) - sP_n(s)]f(s)\}[Q_{n-1}(s) - sQ_n(s)]}{(1-s^2)^2P_n^2(s)}\\ &- \frac{nf(s)[(ns^2 - s^2 - 1)P_n(s) - (2n-3)sP_{n-1}(s) + (n-1)P_{n-2}(s)]}{(1-s^2)^2P_n(s)}.\end{aligned}$$

Example 6.5. Now, we consider an example of less regularity. Let $a = -b = -1$, and $s = 0$ and

$$f(x) = \mathcal{F}_i(x) := x^3 + (2 + \text{sign}(x))|x|^{3-i+0.5}, \quad i = 0, 1.$$

Obviously, $\mathcal{F}_i(x) \in C^{3-i+0.5}[-1, 1](i = 0, 1)$. The exact value of the integral is

$$\mathcal{I}_2(-1, 1; 0, \mathcal{F}_i(x)) = \frac{10-4i}{3-2i}.$$

Here, we use Simpson's rule $\mathcal{Q}_{2n}(s, f)$ and Gaussian method $\mathcal{G}_n(s, f)$ to evaluate the integral. As we all know, if the density function is analytic, the error of Gaussian method decreases very rapidly. But for less regular density function, its accuracy will descend, which can be seen in Table 6. Moreover, also from Table 6, we can see that even for $f(x) \in C^{3-i+\alpha}[-1, 1]$ $(i = 0, 1; \alpha = 0.5)$, the accuracy of Simpson's rule can achieve $O(n^{1-i+\alpha})(i = 0, 1; \alpha = 0.5)$, which show that Simpson's rule is competitive with Gaussian method in this case. More importantly, an advantage of Newton–Cotes rules is their less restriction on the selection of mesh points. In some physical problems, one needs to solve a finite-part integral equation coupled with some domain equations where $f(x)$ is usually unknown and less smooth. The discretization of the integral equation should be made on a mesh which well fits the approximation to the domain equations, such as finite element approximation or finite difference approximation (for example, see [33]). In this case, the composite Newton–Cotes method becomes a competitive one.

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