On a novel numerical quadrature based on cycle index of symmetric group for the Hadamard finite-part integrals

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November 28, 2022

Abstract

To evaluate the Hadamard finite-part integrals accurately, a novel interpolatory-type quadrature is proposed in this article. In our approach, numerical divided difference is utilized to represent the high order derivatives of the integrated function, which make it possible to reduced the numerical quadrature into a concise formula based on the cycle index for symmetric group. In addition, convergence analysis is presented and the error estimation is given. Numerical results are presented on cases with different weight functions, which substantiate the performance of the proposed method.

keyword: Cauchy principal value integral; Hadamard finite-part integral; numerical divided difference; the cycle index of symmetric group.

1 Introduction

The numerical evaluation of Cauchy principal value integrals and Hadamard finite-part integrals has received considerable attention, especially in the boundary element methods[1, 22, 34], where the efficiency of numerical evaluation of such Hadamard finite-part integrals are essential for the boundary element methods. Considering the numerical evaluation of the Hadamard finite-part integrals given by

\[ H_p(\omega; f; \xi) = \int_a^b \omega(x) \frac{f(x)}{(x-\xi)^{p+1}} dx, \quad \xi \in (a, b), \quad p \in \mathbb{N}_0 := \{0, 1, \cdots\}, \quad (1.1) \]

where \( f(x) \) are assumed to be smooth functions and \( \omega(x) \) are nonnegative weight functions on \([a, b]\). In the case of \( p = 0 \), the integral (1.1) is reduced to the well-known Cauchy principal value integral. In this sense, Hadamard finite-part integrals could be also considered as the generalization of Cauchy principal value integrals.

A fundamental idea is to approximate the function \( f(x) \) in (1.1) directly, such as the Lagrange or Lagrange-Hermite interpolation based on a set of distinct nodes. There have been numerous studies on numerical evaluation of integrals with such singularities, such as Gaussian quadrature rule[5, 10, 19, 20, 31], (composite) Newton-Cotes method[15, 16, 17, 32, 35] and some other improved methods[3, 6, 7, 13, 12, 26, 33]. From a theoretical point of view, the above mentioned methods turn out to be convergent only if the function \( f \) is sufficiently smooth.

The main difficulty arising in practical numerical evaluations is the so called "numerical cancellation", which constantly happen when the quadrature nodes approaching the singularity \( \xi \). Considering numerical quadratures, as well as mentioned in [4, 21, 24], subtracting out the singularity from \( f(x) \), (1.1) leads to

\[ H_p(\omega; f; \xi) = \int_a^b \frac{\omega(x)}{(x-\xi)^{p+1}} \left[ f(x) - \sum_{j=0}^{p} \frac{f^{(j)}(\xi)}{j!}(x-\xi)^j \right] dx + \sum_{j=0}^{p} \frac{f^{(j)}(\xi)}{j!} \int_a^b \frac{\omega(x)}{(x-\xi)^{p+1-j}} dx. \quad (1.2) \]

When considering the calculation of above integral, the second part of the right hand side are the Hadamard finite-part integrals, which could be computed analytically with the weight function \( \omega(x) \) known. The first part is

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Hence, the equation (1.2) can be written as the following form
\[ f(x) = \sum_{j=0}^{p} \frac{f^{(j)}(\xi)}{j!} (x - \xi)^j \]

It leads to
\[ f(x) - \sum_{j=0}^{p} \frac{f^{(j)}(\xi)}{j!} (x - \xi)^j = f(x) - \sum_{j=0}^{p} \frac{f(\xi,\ldots,\xi)}{j!} (x - \xi)^j = f[x,\xi^{p+1}](x - \xi)^{p+1}, \]

where \( f[x,\xi^{p+1}] \) denotes the divided difference of the function \( f \) at the points \( x, \xi \), and \( \xi \) is repeated \( p+1 \) times. Hence, the equation (1.2) can be written as the following form
\[
H_p(\omega; f; \xi) = \int_a^b \omega(x) f[x,\xi^{p+1}]dx + \sum_{j=0}^{p} \frac{f^{(j)}(\xi)}{j!} \int_a^b \frac{\omega(x)}{(x - \xi)^{p+1-j}}dx,
\]

where general Gaussian quadrature rule could be applied. Secondly, the proposed quadrature rule can significantly alleviate the difficulty caused by numerical cancellation. Since Lagrange interpolation are calculated based on a different group of nodes, the distances between the nodes \( a_0, a_1, \ldots, a_n \) are large enough so that the computation of the divided differences does not present numerical cancellation.

The rest of the paper is organized as follows. In order to get a explicit result, we need a conception of the cycle index for symmetric group, which is introduced in Section 2. A new quadrature rule for Hadamard finite-part integrals using the numerical divided difference rule is presented in section 3 while a convergent error estimation formula is given in section 4. Finally, we show some numerical examples to illustrate the effectiveness and accuracy in Section 5.

## 2 Cycle index for symmetric group

Let \( \mathfrak{S}_n \) be a symmetric group of degree \( n \) \( (n \in \mathbb{N} = \{1, 2, \ldots\}) \), and for any permutation \( \sigma \in \mathfrak{S}_n \), assume that \( c_i(\sigma) \) is the number of the cycles of length \( i \) in \( \sigma \). Now, we define the cycle index for symmetric group \( \mathfrak{S}_n \) as follows:
\[
Z_n(x_1, x_2, \ldots, x_n) := \frac{1}{|\mathfrak{S}_n|} \sum_{\sigma \in \mathfrak{S}_n} x_1^{c_1(\sigma)} x_2^{c_2(\sigma)} \cdots x_n^{c_n(\sigma)},
\]

where \( |\mathfrak{S}_n| \) represents the order of \( \mathfrak{S}_n \). For convenience, we denote it as
\[
Z_n(x_i) := Z_n(x_i)_{1 \leq i \leq n} := Z_n(x_1, x_2, \ldots, x_n).
\]

As we know \( |\mathfrak{S}_n| = n! \), and the cycle index of the symmetric group can be expressed as the following explicit formulation [2]:
\[
Z_n(x_i) = \sum_{\sigma \in \pi_n} \frac{1}{1^{a_1} a_1! 2^{a_2} a_2! \cdots n^{a_n} a_n!} x_1^{a_1} x_2^{a_2} \cdots x_n^{a_n}, \quad (2.1)
\]
where
\[ \pi_n = \{(a_1, a_2, \ldots, a_n) \in \mathbb{N}_0 \mid 1a_1 + 2a_2 + \cdots + na_n = n\}. \]

In fact, the cycle index of the symmetric group \( Z_n(x_i) \) is a polynomial of degree \( n \) with the variable \( x_1, x_2, \ldots, x_n \). However, it is difficult to obtain the expression from (2.1) for large \( n \), directly. The following recursion relation for \( Z_n(x_i) \) can be easily verified (cf. [25, 27, 30]):

\[
nZ_n(x_i) = \sum_{j=1}^{n} x_j Z_{n-j}(x_i), \quad n \geq 1; \quad Z_0 = 1.
\]

Therefore, we have
\[
Z_1(x) = x_1, \\
Z_2(x) = \frac{1}{2}(x_1^2 + x_2), \\
Z_3(x) = \frac{1}{6}(x_1^3 + 3x_1x_2 + 2x_3), \\
Z_4(x) = \frac{1}{24}(x_1^4 + 6x_1^2x_2 + 3x_2^2 + 8x_1x_3 + 6x_4).
\]

Now, let \( \Omega(x) = \prod_{i=0}^{n}(x - a_i) \), \( g(x) = \log |\Omega(x)| \). Then we have
\[
g^{(k)}(x) = (-1)^{k-1}(k-1)! \sum_{i=0}^{n} (x - a_i)^{-k}, \quad x \neq a_i (i = 0, 1, \ldots, n).
\]

This is together with Faà di Bruno’s formula
\[
\frac{d^k}{dx^k} \exp(g(x)) = k! \exp(g(x)) Z_k \left( \frac{g^{(r)}(x)}{(r-1)!} \right).
\]

**Lemma 2.1** Assume that \( a_0, a_1, \ldots, a_n \) are distinct points, then we have
\[
\frac{1}{k!} \Omega^{(k)}(x) = \Omega(x)Z_k(-S_r(x)), \quad S_r(x) = \sum_{i=0}^{n} \frac{1}{(a_i - x)^r} x \neq a_i.
\]

Especially,
\[
\frac{1}{k!} \Omega^{(k)}(x) \bigg|_{x=a_i} = \Omega'(a_i)Z_{k-1}(-S_{ri}(a_i)), \quad S_{ri}(x) = \sum_{j=0}^{n} \frac{1}{(a_j - x)^r}.
\]

**Proof.** For \( x \neq a_i \),
\[
\Omega^{(k)}(x) = \frac{d^k}{dx^k} (\text{sgn}(x) \exp(g(x))) = k! \Omega(x) Z_k \left( \frac{g^{(r)}(x)}{(r-1)!} \right),
\]

together with (2.2), we obtain (2.3).

For \( x = a_i \), according to the Leibnitz formula for high order derivatives,
\[
\frac{d^k}{dx^k} (\frac{\Omega(x)}{x-a_i}) = k! \Omega(x) Z_k(-S_{ri}(x)) + \frac{\Omega(x)}{x-a_i} Z_{k-1}(-S_{ri}(x)).
\]

Applying \( \Omega(a_i) = 0 \) and \( \frac{\Omega(x)}{x-a_i} \bigg|_{x=a_i} = \Omega'(a_i) \), we complete the proof. \( \square \)

The next theorem is verified from Lemma 2.1.
Theorem 2.1 We denote by \( l_i(x) \) the Lagrange fundamental polynomial interpolating at the points \( a_0, a_1, \cdots, a_n \),

\[
l_i(x) = \frac{\Omega(x)}{(x-a_i)\Omega'(a_i)}.
\]

For \( x \neq a_j \) (\( j \neq i \)), we have

\[
\frac{1}{k!} f^{(k)}(x) = l_i(x)Z_k(-S_{rij}(x)). \tag{2.4}
\]

In particular for \( x = a_j \) (\( j \neq i \)), the following equation holds,

\[
\frac{1}{k!} f^{(k)}(x) = l'_i(a_j)Z_{k-1}(-S_{rij}(x)), \quad S_{rij}(x) = \sum_{l=0}^{n} \frac{1}{(a_l - x)^r}. \tag{2.5}
\]

**Proof.** Due to \( l_i(x) = \frac{1}{\Omega'(a_i)} \prod_{j=0 \atop j \neq i}^{n} (x-a_j) \), we obtain (2.4) combined with (2.3).

For \( x = a_j \) (\( j \neq i \)), following from the Leibnitz formula,

\[
l_i^{(k)}(x) = (x-a_j) \left( \frac{l_i(x)}{(x-a_j)} \right)^{(k)} + k \left( \frac{l_i(x)}{(x-a_j)} \right)^{(k-1)}
\]

\[
= k!l_i(x)Z_k \left( -\sum_{l=0 \atop l \neq i,j}^{n} \frac{1}{(a_l - x)^r} \right) + k! \frac{l_i(x)}{(x-a_j)}Z_{k-1} \left( -\sum_{l=0 \atop l \neq i,j}^{n} \frac{1}{(a_l - x)^r} \right).
\]

Applying \( l_i(a_j) = 0 \) (\( j \neq i \)), (2.5) holds and the proof is completed. \( \square \)

3 Quadrature formula

Let \( x_1, x_2, \cdots, x_m \) be quadrature nodes on \([a, b]\), which is based on the zeros of the orthonormal polynomial with respect to the weight \( \omega(x) \). Gaussian quadrature rule is applied to the fist integral on the right hand of (1.3), which leads to

\[
H_m(\omega; f; \xi) = \sum_{k=1}^{m} \lambda_k f[x_k, \xi^{p+1}] + \sum_{j=0}^{p} \frac{f^{(j)}(\xi)}{j!} \int_{-\xi}^{b} \frac{\omega(x)}{(x-\xi)^{p+1-j}} dx. \tag{3.1}
\]

The divided differences \( f[x_k, \xi^{p+1}] \) are obtained making use of the value of function \( f \) at \( x_k \) and \( \xi \). However, when \( x_k \) is very close to the singularity \( \xi \), the practical evaluation will produce large rounding errors due to numerical cancellation. Therefore, it is expected that the distance between \( x_k \) and \( \xi \) is large enough. But how to define "very close" and "large enough"? For example, let \( x_c \) be the quadrature node closest to \( \xi \), then the distances of the rest quadrature nodes to \( \xi \) are considered to be large enough. That is, for any fixed \( \xi \), \( x_c \) is defined by

\[
|\xi - x_c| = \min \{ |\xi - x_k|, k = 1, 2, \ldots, m \},
\]

when \( \xi \) is equidistant between two zeros, i.e., \( \xi = \frac{1}{2}(x_k + x_{k+1}) \) for some \( k \in \{1, 2, \ldots, m - 1\} \), then we choose two nodes \( x_c = x_k \) and \( x_c = x_{k+1} \).

In this case, there is an effective way to calculate \( f[x_k, \xi^{p+1}] \) proposed by X. H. Wang, H. Y. Wang and M. J. Lai[29], where the divided differences of the interpolation of \( f \) is used to approximate the divided differences of \( f \). The divided differences \( f[x_k, \xi^{p+1}] \) can be calculated easily without producing numerical cancellation expect \( f[x_c, \xi^{p+1}] \). For \( f[x_c, \xi^{p+1}] \) we can use the divided differences of the interpolation of \( f \) on another group of nodes \( a_0, a_1, \cdots, a_n \) and the distances between the nodes are large enough. We assume that \( a_0, a_1, \cdots, a_n \) are quasi-uniform nodes, that is, there exists constant \( c > 0 \) such that

\[
\max \{ \pi_{i+1} - \pi_i | 0 \leq i < n \} \leq cd.
\]

Here \( \pi_0 < \pi_1 < \cdots < \pi_n \) is the rearrangement of \( a_0, a_1, \cdots, a_n \) and \( d \) is defined by

\[
d = \min \{ \pi_{i+1} - \pi_i | 0 \leq i < n \},
\]
obviously, we need \( x_c, \xi \in [\pi_0, \pi_n] \) and \( d > |x_c - \xi| \).

Furthermore, how to choose the nodes \( a_0, a_1, \cdots, a_n \) is also an important problem. Actually, in numerical computing practice, we choose the equidistant nodes in the interval \([a, b]\) and let \( \xi \) be one of the nodes. For instance \( b - \xi < \xi - a \), then we suppose that the subinterval \([\xi, b]\) is divided into \( \nu + 1 \) parts and let \( h = \frac{b-\xi}{\nu+1} \) be step. In the subinterval \([a, \xi]\), it is divided into \( n - \nu \) parts under the step \( h \).

\[
\begin{align*}
a_0 &= \xi, a_1 = \xi + h, a_3 = \xi + 2h, \cdots, a_{2\nu-1} = \xi + \nu h, \\
a_2 &= \xi - h, a_4 = \xi - 2h, \cdots, a_{2\nu} = \xi - \nu h, \\
a_{2\nu+1} &= \xi - (\nu + 1)h, a_{2\nu+2} = \xi - (\nu + 2)h, \cdots, a_n = \xi - (n - \nu)h.
\end{align*}
\]

(3.2)

It requires \( n \geq 2\nu \) and \( a_n = \xi - (n - \nu)h > a \) to ensure the most information are used and all nodes are inside \([a, b]\). This needs

\[
\frac{a - \xi + n(b - \xi)}{b - a} < \nu \leq \frac{n}{2}.
\]

Hence, once the number of nodes \( n \) is conformed, the nodes \( a_0, a_1, \cdots, a_n \) are conformed too.

Now, we can construct Lagrange interpolation polynomial at these nodes. Assume that \( L_n(x) \) is the Lagrange polynomial which interpolates the function \( f \) at \( a_0, a_1, \cdots, a_n \) and written as

\[
L_n(x) = \sum_{i=0}^{n} l_i(x)f(a_i),
\]

where \( l_i(x) \) is the Lagrange fundamental polynomial mentioned in Theorem 2.1. The divided difference of the interpolate polynomial \( L_n(x) \) at the points \( x \) and \( \xi \) is obtained, where \( \xi \) is repeated \( p + 1 \) times,

\[
L_n[x, \xi^{p+1}] = \sum_{i=0}^{n} l_i[x, \xi^{p+1}]f(a_i).
\]

Observe that \( l_j(x) \) is a polynomial of degree \( n \), and the following property of the divided difference is an easy exercise:

\[
l_i[x, \xi^{p+1}] = \frac{1}{(x - \xi)^{p+1}} \left( l_i(x) - \sum_{k=0}^{p} \frac{l_i^{(k)}(\xi)}{k!} (x - \xi)^k \right)
\]

\[
= \frac{1}{(x - \xi)^{p+1}} \left( l_i(\xi) + l_i'(\xi)(x - \xi) + \cdots + \frac{l_i^{(n)}(\xi)}{n!} (x - \xi)^n - \sum_{k=0}^{p} \frac{l_i^{(k)}(\xi)}{k!} (x - \xi)^k \right)
\]

\[
= \sum_{k=p+1}^{n} \frac{l_i^{(k)}(\xi)}{k!} (x - \xi)^{k-p-1}.
\]

Therefore, the divided difference \( f[x_c, \xi^{p+1}] \) can be rewritten as

\[
f[x_c, \xi^{p+1}] \approx L_n[x_c, \xi^{p+1}] = \sum_{i=0}^{n} f(a_i) \sum_{k=p+1}^{n} \frac{l_i^{(k)}(\xi)}{k!} (x_c - \xi)^{k-p-1}.
\]

(3.3)

Theorem 3.1 Let \( A_i^{(k)} = \frac{l_i^{(k)}(\xi)}{k!}, \) nodes \( a_0, a_1, \cdots, a_n \) are given by (3.2), then from Theorem 2.1 we have

\[
A_0^{(k)} = Z_k(\eta_r), \quad \eta_r = -\frac{1}{hr} \left[ \sum_{j=1}^{\nu} \frac{1}{j^r} + \sum_{j=1}^{n-\nu} \frac{(-j)^r}{j^r} \right],
\]

(3.4)

For \( i = 1, 2, \cdots, \nu \), the following formulae hold

\[
A_{2i-1}^{(k)} = \frac{(-1)^{i-1} \nu (n - \nu)!}{h(\nu - i)! (n - \nu + i)!} Z_{k-1} \left( \eta_r + \frac{1}{hr} \right),
\]

\[
A_{2i}^{(k)} = \frac{(-1)^i \nu! (n - \nu)!}{h(\nu + i)! (n - \nu - i)!} Z_{k-1} \left( \eta_r + \frac{1}{hr} \right),
\]

For \( i = 1, 2, \cdots, \nu \), the following formulae hold

\[
A_{2i-1}^{(k)} = \frac{(-1)^{i-1} \nu (n - \nu)!}{h(\nu - i)! (n - \nu + i)!} Z_{k-1} \left( \eta_r + \frac{1}{hr} \right),
\]

\[
A_{2i}^{(k)} = \frac{(-1)^i \nu! (n - \nu)!}{h(\nu + i)! (n - \nu - i)!} Z_{k-1} \left( \eta_r + \frac{1}{hr} \right),
\]

(3.4)
and for \( i = \nu + 1, \nu + 2, \cdots, n - \nu \), it follows as

\[
A_{i+1}^{(k)} = \frac{(-1)^i \nu! (n-\nu)!}{h^i (\nu + i)! (n-\nu - i)!} Z_{k-1} \left( \eta_r + \frac{1}{h r (-i)^r} \right).
\]

**Proof.** Since \( \xi = a_0 \), this enables us to use equation (2.4), we have

\[
A_0^{(k)} = \frac{i_0^{(k)} (\xi)}{k!} = Z_k (-S_{r0}(a_0)).
\]

From (3.2), the following equation can be easily verified

\[-S_{r0}(a_0) = -\sum_{j=1}^{n} \frac{1}{(a_j - a_0)^r} \]

\[-\left[ \sum_{j=1}^{\nu} \frac{1}{(a_{2j-1} - a_0)^r} + \frac{1}{(a_{2j} - a_0)^r} \right] + \sum_{j=2\nu+1}^{n} \frac{1}{(a_j - a_0)^r} \]

\[-\frac{1}{h r} \left[ \sum_{i=1}^{\nu} \frac{1}{i^r} + \sum_{i=1}^{n-\nu} \frac{1}{(-i)^r} \right] = \eta_r,
\]

and this immediately infers (3.5). For \( i = 1, 2, \cdots, \nu \) and from (2.5) \( A_i^{(k)} = i' \xi Z_{k-1} (-S_{r0}(\xi)) \), it is easy to verify that

\[i'_{2i-1} (\xi) = \frac{(-1)(-2) \cdots (-i+1)(-i-1) \cdots (-\nu) \cdot 1 \cdot 2 \cdots (n-\nu) h^{n-1}}{i(i-1) \cdots 1(-1)(-2) \cdots (i-\nu)(i+1) \cdots (i+n-\nu) h^n}
\]

\[= \frac{(-1)^{i-1} \nu! (n-\nu)!}{i h (\nu - i)! (n - \nu + i)!}.
\]

Furthermore,

\[S_{r,2i-1,0} (\xi) = \sum_{j=1}^{\nu} \frac{1}{(a_{2j-1} - a_0)^r} + \sum_{j=1}^{\nu} \frac{1}{(a_{2j} - a_0)^r} + \sum_{j=2\nu+1}^{n} \frac{1}{(a_j - a_0)^r} \]

\[= \frac{1}{h r} \left( \sum_{i=1}^{\nu} \frac{1}{j^r} + \sum_{i=1}^{n-\nu} \frac{1}{(-j)^r} \right) = -\eta_r - \frac{1}{h r^r},
\]

Together with \( i'_{2i-1} (\xi) \), we get \( A_{2i-1}^{(k)} \). In the case of \( A_{2i}^{(k)} \) and \( A_{\nu+1}^{(k)} \), can be obtained in a similar way. The proof is completed.

Combining equation (3.1), (3.3) and Theorem 3.1, we finally achieve the formula

\[H_{m, n, p} (\omega; f; \xi) = \sum_{k=1}^{m} \lambda_k f(x_k, \xi^{p+1}) + \lambda_c \sum_{i=0}^{n} f(a_i) \sum_{k=p+1}^{n} A_i^{(k)} (x_c - \xi)^{k-p-1} \]

\[+ \sum_{j=0}^{p} \frac{f^{(j)} (\xi)}{j!} \int_{a}^{b} \frac{\omega(x)}{(x - \xi)^{p+1-j}} dx.
\]

It is worth to remark that the complexity of numerical quadrature proposed here is better than traditional method. It takes account of high order information and has the advantage that the coefficients could be calculated in a recurrent manner, which is usually stable and efficient in practical numerical calculations. Take \( A_{2i-1}^{(k)} \) as example, we could calculate it in two steps. Firstly we calculate

\[x_r := \eta_r + \frac{1}{h r^r} = \frac{1}{h r \sum_{j=1}^{\nu} \frac{1}{j^r} + \sum_{j=1}^{n-\nu} \frac{1}{(-j)^r} + \frac{1}{i^r}} (r = 1, 2, \cdots, k - 1)
\]
with $\sum_{r=1}^{k-1} (n+2)(r-1) = O(k^2)$ multiplication operations (n is a fixed number). In the second step, the recurrence relation $(k-1)Z_{k-1}(x_r) = \sum_{j=k-1}^{n} x_j Z_{k-j-1}(x_r)$, $Z_0 = 1$ with $1 + 2 + \cdots + k - 1 = O(k^2)$ multiplication operations is applied. Based on the above analysis, it is known that the solution of $A_{(k)}^{(i)}$ requires only $O(k^2)$ operations.

As the comparison, let us show that traditional scheme for calculating $A_{(k)}^{(i)} = \frac{I_i^{(k)}(\xi)}{k!}$ cost more than the one using cycle index. Notice that

$$I_i^{(k)}(x) = \prod_{j=0}^{n} \frac{x - a_j}{a_i - a_j} = (\prod_{j=0, j \neq i}^{n} \frac{1}{a_i - a_j}) \phi_n(x), \quad \phi_n(x) := \prod_{j=0}^{n} (x - a_j).$$

According to Leibniz formula,

$$\phi_n^{(k)}(x) = \sum_{m_0 + m_1 + \cdots + m_n = k} \frac{k!}{m_0! m_1! \cdots m_n!} \prod_{j=0}^{n} (x - a_j)^{(m_j)}$$

$$= k! \sum_{0 \leq j_0 \leq j_1 \leq \cdots \leq j_{n-k} \leq n} \prod_{j=0}^{n-k} (x - a_{j_i}),$$

where we only consider the case that $m_j$ equals to 0 or 1 (when $m_j \geq 2$, $(x - a_j)^{(m_j)} \equiv 0$), thus the number of zero-valued $m_j$ is $(n - k + 1)$, and their subscripts are denoted as $j_0, j_1, \ldots, j_{n-k}$. Once all the combinations of $a_{j_i}$ are determined, we get the result of $A_{(k)}^{(i)}$. It’s easy to verify that the above process requires $\binom{n+1}{k}(n - k)$ operations (n is a fixed number), which is much more than $O(k^2)$.

4 Error analysis

In this section, we estimate the error of the quadrature formula in (3.5). The remainder term of the Gaussian quadrature formula (3.1) with the nodes $x_1, x_2, \cdots, x_n$ is denoted as $R_m(g)$ where $g(x) = f[x, \xi^{p+1}]$, while the remainder term in polynomial interpolation with the nodes $a_0, a_1, \cdots, a_n$ is denoted as $R_n[x, \xi^{p+1}]$. The value $m$ and $n$ are given independently.

Lemma 4.1 Let $\Gamma$ be a simple closed curve in the complex plane surrounding the interval [-1,1] and D its interior. Having been subtracted out the singularity, the integrand $g$ is an analytic function in D, thus the remainder term $R_m(g)$ admits the contour integral representation (cf. [18])

$$\frac{1}{2\pi i} \oint_{\Gamma} K_m(z) g(z) dz. \quad (4.1)$$

The kernel $K_m(z)$ is given by $K_m(z) = \frac{\rho_m(z)}{\pi m(z)}$, where $\rho_m(z) = \int_{-1}^{1} \omega(t) \frac{\pi_m(t)}{z - t} dt$, and $\pi_m(t)$ is the corresponding orthogonal polynomial with respect to the weight function $\omega(t)$ on (-1,1).

Lemma 4.2 Take the contour $\Gamma$ as a confocal ellipse with foci at the points -1, +1 and sum of semi-axes $\rho > 1$, $\varepsilon_\rho = \{ z \in \mathbb{C} : z = \frac{1}{2}(\rho e^{i\theta} + \rho^{-1} e^{-i\theta}), 0 \leq \theta \leq 2\pi \}$. D. B. Hunter (cf. [9]) gives the expansion of $\rho_m(z)$ and $\pi_m(z)$ defined in (4.1), together with an error estimation inequality as follows:

$$|R_m(g)| \leq \frac{4M(\varepsilon_\rho)}{\rho^{2m-1}(\rho - 1)} \int_{-1}^{1} \omega(t) dt, \quad (4.2)$$

where $M(\varepsilon_\rho) = \max_{z \in \varepsilon_\rho} |g(z)|$. Note that for certain specific weight functions, the above error bound can be further improved. For example, N. S. Kambo (cf. [11]) gives the error bound of Gauss-Legendre quadrature formulae as $|R_m(g)| \leq \frac{\pi M(\varepsilon_\rho)(\rho^2 + 1)}{\rho^{2m}(\rho^2 - 2)}$, which is better than (4.2) if $\rho$ is large ($\rho > \sqrt{2}$).
Lemma 4.3 Assume that \( x_0, x_1, \ldots, x_k \) and \( a_0, a_1, \ldots, a_n \) are sequences of nodes in \( \mathbb{R} \) or in \( \mathbb{C} \) (\( k \leq n \)). Then for any integer \( m \) satisfying \( 0 \leq m \leq k \), the divided difference of the remainder in polynomial interpolation can be expressed as (cf. [28])

\[
R[x_0, x_1, \ldots, x_k] = \sum_{v=0}^{m-1} f[x_0, x_1, \ldots, x_v, a_0, a_1, \ldots, a_n] \omega_{v+1}[x_v, x_{v+1}, \ldots, x_k]
\]

\[
+ \sum_{v=m}^{k} f[x_0, x_1, \ldots, x_v, a_0, a_1, \ldots, a_n + m - v](x_v - a_{n + m - v}) \omega_{n + m - v}[x_v, x_{v+1}, \ldots, x_k],
\]

where \( v = 0, 1, \ldots, n + 1 \), and

\[
\omega_v(x) := \prod_{i=0}^{v-1} (x - a_i), \quad R(x) := f(x) - \sum_{v=0}^{n} f[a_0, a_1, \ldots, a_v] \omega_v(x).
\]

Lemma 4.4 The sequences of nodes \( x_0, x_1, \ldots, x_k \) and \( a_0, a_1, \ldots, a_n \) are defined in Lemma 4.3, then

\[
(f[x_0, x_1, \ldots, x_k, x])[a_0, a_1, \ldots, a_n] = f[x_0, x_1, \ldots, x_k, a_0, a_1, \ldots, a_n].
\]

We can use the definition of divided difference and apply traditional mathematics inductive approach to prove this lemma.

Theorem 4.1 Suppose that \( f \in \mathbb{C}^{n+2}[-1, 1] \), \( f^{(n+1)}, f^{(n+2)} \) are bounded, and \( a_0, a_1, \ldots, a_n \) are given in (3.2), \( n > p \). Meanwhile, \( x_1, x_2, \ldots, x_m \) are chosen as the Gauss-Jacobi nodes with respect to the weight \( \omega(t) = (1-t)^\alpha(1+t)^\beta \) on \((-1, 1)\) and \( \rho, M(\varepsilon_\rho) \) are defined in Lemma 4.2. Then we have the error estimation formula

\[
|R_{m,n}| \leq \frac{2^{n+\beta+3}\Gamma(\alpha+1)\Gamma(\beta+1)M(\varepsilon_\rho)}{\Gamma(\alpha+\beta+2)\rho^{2m-1}(\rho-1)} + \frac{M_1 + M_2}{(n-p)!}(1 + \frac{p + 2}{n})^{n-p}.
\]

where \( M_1 = \max |f^{(n+1)}|, M_2 = \max |f^{(n+2)}| \).

Proof. Substituting the weight function \( \omega(t) = (1-t)^\alpha(1+t)^\beta \) into (4.2), we obtain that

\[
|R_m(g)| \leq \frac{2^{n+\beta+3}\Gamma(\alpha+1)\Gamma(\beta+1)M(\varepsilon_\rho)}{\Gamma(\alpha+\beta+2)\rho^{2m-1}(\rho-1)},
\]

In practice, \( M(\varepsilon_\rho) \) is calculated for several values of \( \rho \) within the appropriate range and the smallest number so obtained is taken as the upper bound for \( R_m(g) \). Once \( \alpha, \beta, \rho \) are fixed and \( m \to \infty \), we get \( R_m(g) \to 0 \).

According to the definition of the remainder term in polynomial interpolation,

\[
R_n[x, \xi^{p+1}] = f[x, \xi^{p+1}] - \sum_{v=0}^{n} f[a_0, a_1, \ldots, a_v] \omega_v[x, \xi^{p+1}].
\]

From Lemma 4.3, \( a_0, \beta_0, a_v \in (-1, 1) \), we know that

\[
R_n[x, \xi^{p+1}] = R[x, \xi^{p+1}] = f[x, a_0, a_1, \ldots, a_n] \omega_{n+1}[x, \xi^{p+1}]
\]

\[
+ \sum_{v=1}^{p+1} f[x, \xi^v, a_0, a_1, \ldots, a_{n+1-v}] \omega_{n+1-v}[\xi^{p+2-v}]
\]

\[
= f^{(n+1)}(a_0) \omega_{n+1}[\xi^0] + \sum_{v=1}^{p+1} f^{(n+2)}(a_v) \omega_{n+1-v}[\xi^{p+1-v}],
\]

From Leibniz formula,

\[
\omega_{n+1}^{(k)}(x) = \sum_{m_0 + m_1 + \ldots + m_k = k} \frac{k!}{m_0!m_1! \ldots m_k!} \prod_{j=0}^{n} (x - \alpha_j)^{(m_j)}
\]

\[
= k! \sum_{0 \leq j_0 < j_1 < \ldots < j_{n-k} \leq n} \prod_{i=0}^{n-k} (x - \alpha_j_i).
\]
Let $a_j = \xi - \lambda_j h, h = \frac{1 - \xi}{n+1}$ (defined in (3.2)), where
\[-\nu \leq \lambda_j \leq n - \nu, \nu > \frac{-1 - n(1 - \xi)}{2},\]
thus we obtain $h < \frac{2}{n+1}$, and then
\[
\prod_{i=0}^{n-k} (x - a_i) \leq \left( \sum_{i=0}^{n-k} (x - \xi + \lambda_j h) \right)^{n-k+1}
\leq \left( \frac{(n - k + 1)(x - \xi) + (\sum_{i=0}^{n-k} \lambda_j)h}{n - k + 1} \right)^{n-k+1}
\leq \left( \frac{(n - k + 1)(x - \xi) + (\sum_{i=0}^{n-k} \lambda_j h)}{n - k + 1} \right)^{n-k+1}
\leq \left( 1 - \xi + \frac{n + k - 2\nu}{2} h \right)^{n-k+1} = \left( \nu + 1 + \frac{n + k - 2\nu}{2} \right)^{n-k+1} h^{n-k+1}
= \frac{(n + k + 2)^{n-k+1}}{n+1} h^{n-k+1} \leq \left( 1 + \frac{k + 1}{n+1} \right)^{n-k+1},
\]
so we get $\omega_n^{(k)}(x) \leq k! (\frac{n+1}{n+1})(1 + \frac{k+1}{n+1})^{n-k+1}$. Therefore,
\[
|R_n[x, \xi^{p+1}]| \leq \frac{|f^{(n+1)}(a_0)|}{(n+1)!} \omega_n^{(p+1)}(\beta_0) + \sum_{v=1}^{p+1} \frac{|f^{(n+2)}(a_v)|}{(n+2)!} (\xi - a_{n+1-v}) \omega_n^{(p+1-v)}(\xi)\frac{(p+1-v)!}{(p+1-v)!}
\leq \frac{M_1}{(n+1)! (p+1)! (n-p)!} (1 + \frac{p + 2}{n+1})^{n-p} + \sum_{v=1}^{p+1} \frac{M_2}{(n+2)!} (n-v) \left( \frac{n+1-v}{p+1-v} \right)^{n-p}
\leq \frac{M_1}{(n+1)! (p+1)! (n-p)!} (1 + \frac{p + 2}{n+1})^{n-p} + \sum_{v=1}^{p+1} \frac{M_2}{(n+2)!} (n-v) \left( \frac{n+1-v}{p+1-v} \right)^{n-p}
\leq \frac{M_1}{p! (n-p)!} (1 + \frac{p + 2}{n+1})^{n-p} + \frac{M_2}{p! (n-p)!} (n-v) \left( \frac{n+1-v}{p+1-v} \right)^{n-p}
\leq \frac{M_1 + M_2}{p! (n-p)!} (1 + \frac{p + 2}{n+1})^{n-p}.
\]
Once $p$ is fixed and $n \to \infty$, $(1 + \frac{p+2}{n+1})^{n-p} \to e^{p+2}$, where $e$ is the base of natural logarithms, thus we get $R_n[x, \xi^{p+1}] \to 0$. Therefore, the convergence of the error estimation formula has been proved.

5 Numerical Examples

In this section, we present some numerical examples to demonstrate the applicability and accuracy of the quadrature rule proposed in this paper. In the quadrature formula (3.5), $x_1, x_2, \cdots, x_m$ are chosen as the Gaussian nodes with respect to the weight $\omega(x)$. Furthermore, the formula involves another group of nodes $a_0, a_1, \cdots, a_n$. Here absolute error is defined as the absolute value of the true error and the missing points in the figures indicate that the data have reached machine precision. Note that all computations carried out in this paper were performed using the package of MATLAB 2017b on a personal computer with the operating system Windows 10, 8 GB RAM and 2.11 GHz CPU clock speed.

Example 5.1 Here, we give the following Hadamard finite-part integral to verify some properties of the new quadrature rule.
\[
I_1(\xi; p) = \int_{-1}^{1} \frac{e^x}{(x - \xi)^{p+1}} dx,
\]
where \( x_1, x_2, \ldots, x_m \) are zeros of Legendre polynomial.

If \( p = 0 \), the exact solution of the above integral can be expressed as

\[
[Ei(1 - \xi) - Ei(-1 - \xi)]e^\xi,
\]

where \( Ei(x) = \int_{-\infty}^{x} \frac{e^t}{t} \, dt \) represents the exponential integral. Once we fix the value of \( m \) and \( n \), the absolute errors of the approximations to \( I_1(\xi; p) \) can be obtained for different singularities. From Figure 1, we observe that the error is bounded uniformly, namely, independently of \( \xi \), which is an illustrative evidence of uniform error bound mentioned in Section 4.

![Figure 1: the absolute errors of the approximations to \( I_1(p = 0, m = 7, n = 8) \) for different singularities \( \xi \)]

When \( \xi = 10^{-5} \), we present the absolute errors \( R_{m,n}^* \) of \( I_1 \) in Table 1 with varied values of \( n \) and different numbers of quadrature nodes \( m \), where \( p \) is given by 0 and 1. Meanwhile, we also record the execution time of our algorithm for each \( m \) and \( n \) (take the average of ten measurements). From this table, we can see that for both \( p = 0 \) and \( p = 1 \), the error decreases sharply at the beginning while \( n \) is increasing but when \( n \) is large enough the error fluctuates up and down in a small range or even rises up. We can also see this phenomenon on the left figure of Figure 2. Meanwhile, a bigger \( n \) will lead to longer execution time for our algorithm (see Figure 3).

| Table 1: the absolute errors \( R_{m,n}^* \) of \( I_1(\xi = 10^{-5}) \) for \( p = 0 \) and \( p = 1 \) |
|---|---|---|---|---|
| \( n \) | \( R_{m,n}^*(m = 7) \) | \( R_{m,n}^*(m = 15) \) | \( R_{m,n}^*(m = 7) \) | \( R_{m,n}^*(m = 15) \) |
| 4 | 1.742840E - 04 | 8.447273E - 05 | 2.897117E - 05 | 1.404187E - 05 |
| 8 | 1.716980E - 09 | 8.321455E - 10 | 1.719901E - 10 | 8.335765E - 11 |
| 11 | 1.940670E - 13 | 9.281464E - 14 | 2.134959E - 13 | 1.051381E - 13 |
| 12 | 3.108624E - 15 | 3.108624E - 15 | 6.328271E - 15 | 1.665335E - 15 |
| 24 | 4.440892E - 16 | 1.776357E - 15 | 1.765254E - 16 | 1.110223E - 16 |
| 31 | 2.664535E - 15 | 1.332267E - 15 | 4.107825E - 15 | 3.885781E - 15 |
| 44 | 2.220446E - 15 | 2.220446E - 15 | 1.221245E - 15 | 2.409184E - 14 |
| 59 | 3.996803E - 15 | 1.776357E - 15 | 1.282308E - 13 | 6.694645E - 14 |

Therefore we’re supposed to find an optimal option of \( n = \hat{n} \) which makes the error relatively small. In Figure 2, we find that when taking different values of \( m \), the value of \( n \) tends to be stable. In particular when \( m \) takes a larger number, the absolute errors increase. To reduce the execution time effectively, we can take the above stable value \( n \) as an optimal value \( \hat{n} \), especially when \( m \) is relatively large. For small values of \( m \), like those less than or closer to the stable value \( n \), we can limit the search to a certain small range \([m - \delta, m + \delta]\). For instance, when \( m = 15, \delta = 10 \) for \( p = 0 \) and \( p = 1 \) it’s easy to calculate by MATLAB that \( \hat{n} \) equals to 25 and 15, respectively (see Figure 3).

**Example 5.2** In this example, we show numerical results for the following Hadamard finite-part integral:

\[
I_2 = \int_{-1}^{1} \frac{(1.21 - x^2)^{-1/2}}{(x - 10^{-5})^2} \, dx.
\]
Figure 2: the absolute errors of the approximations to $I_1(p = 1)$ for different $n$ and $m$

Figure 3: the absolute errors and execution time of the approximations to $I_1(m = 15, \xi = 10^{-5})$ for different value $p$

In this case $\omega(x) = 1$, so that $x_m$ are zeros of Legendre polynomial and the exact solution of $I_2$ is $-0.757450528292818$.

Firstly we make certain an appropriate value $n = \hat{n}$ for each $m$. It can be discovered from Figure 5 that for a fixed $m$, the error curve will not decline continuously when $n$ is large enough, thus $\hat{n}$ can be determined using the method mentioned in the last experiment.

Then we compare numerically the quadrature formula (3.5) (denoted as Algorithm 3) with the Gaussian quadrature formula considered in [10] and another quadrature formula proposed in [3] (denoted as Algorithm 1 and Algorithm 2 respectively). Some results are shown in Table 2. We see that our new quadrature rule converges much faster and has higher rate of convergence. The only disadvantage is the longer execution time. The main reason for the longer time is that it takes more time to search the optimal $n$ value. But we can reduce it efficiently by using the stable value $n$ for bigger $m$, which might not be the best option but makes the absolute error have the same order of magnitude as the best situation.

| Algorithm 1 | Algorithm 2 | Algorithm 3 |
|-------------|-------------|-------------|
| $m$ | absolute error | time(s) | absolute error | time(s) | absolute error | time(s) |
| 3 | 3.926491E−02 | 0.4991 | 1.768617E−01 | 0.0851 | 2.359030E−02 | 0.2786 |
| 9 | 1.239733E−04 | 0.6375 | 9.282299E−03 | 0.0862 | 1.047047E−04 | 0.7463 |
| 15 | 1.541521E−07 | 0.7231 | 4.928689E−04 | 0.0868 | 5.776838E−08 | 1.2668 |
| 21 | 2.980971E−06 | 0.8336 | 2.900791E−05 | 0.0870 | 1.792015E−09 | 2.1794 |
| 27 | 4.032681E−06 | 1.0016 | 1.781499E−06 | 0.1022 | 2.230882E−12 | 2.9998 |
| 33 | 3.435934E−06 | 1.2002 | 1.123160E−07 | 0.1215 | 4.853014E−14 | 6.8992 |
| 39 | 1.207606E−06 | 1.4634 | 7.204918E−09 | 0.1331 | 9.325873E−15 | 12.3193 |
| 45 | 3.254382E−06 | 2.4647 | 4.679410E−10 | 0.1484 | 7.105427E−15 | 18.1009 |
Figure 4: the absolute errors of the approximations to $I_2$ for different $n$ and the best option of $n = \hat{n}$ for each $m$

**Example 5.3** In this example, we show numerical results for the following Hadamard finite-part integral:

$$I_3(\xi, \lambda) = \int_{-1}^{1} \frac{(x^2 + \lambda^2)^{-1}}{(x - \xi)\sqrt{1 - x^2}} \, dx, \quad \xi = 0.25.$$  

In this case $\omega(x) = 1/\sqrt{1 - x^2}$, so that $x_m$ are zeros of Chebyshev polynomial of the first kind and the exact solution of $I_3(\xi, \lambda)$ is

$$\frac{\pi(\xi^2 - \lambda^2)}{\lambda \sqrt{\lambda^2 + 1(\lambda^2 + \xi^2)}}.$$  

In this example, we present the absolute errors $R_m^*$ of $I_3$ in Table 3 with varied values of $\lambda$ (so that the integrand functions differ from each other). It can be discovered that for a bigger value $\lambda$ we have a higher rate of convergence in our quadrature formula. Then we compare numerically our method with the quadrature formula proposed in [3] and show the results in Figure 5. For varied values of $\lambda$, the quadrature formula (3.5) is of higher accuracy than the other method.

| $\lambda$ | $m$ | $n$ | $R_m^*$ | $\hat{n}$ | $R_{\hat{n}}$ | $\tilde{n}$ | $R_{\tilde{n}}$ |
|---|---|---|---|---|---|---|---|
| 1.5 | 3 | 5 | 4.638894E − 04 | 10 | 7.395720E − 06 | 10 | 9.222675E − 09 |
| 4 | 6 | 2.586007E − 06 | 6 | 2.677880E − 07 | 10 | 9.052034E − 11 |
| 5 | 14 | 6.152098E − 06 | 19 | 9.831182E − 09 | 16 | 1.001525E − 13 |
| 8 | 10 | 2.894122E − 07 | 10 | 1.404692E − 11 | 12 | 8.596422E − 15 |
| 7 | 12 | 2.906012E − 08 | 13 | 4.271375E − 12 | 14 | 4.796510E − 16 |
| 8 | 20 | 4.742672E − 09 | 18 | 5.149353E − 13 | 23 | 4.510281E − 17 |
| 9 | 21 | 4.349271E − 10 | 21 | 9.450773E − 15 | 15 | 1.734723E − 17 |
| 10 | 21 | 4.008799E − 11 | 21 | 4.857226E − 16 | 15 | 4.423545E − 17 |
| 11 | 22 | 3.663181E − 12 | 22 | 6.661338E − 16 | 12 | 1.908196E − 17 |
| 12 | 21 | 4.963807E − 13 | 20 | 9.992007E − 16 | 17 | 8.073617E − 19 |

Table 3: the absolute errors $R_m^*$ of $I_3(\xi = 0.25)$ for different values of $\lambda$

We have presented efficient method for the computation of Cauchy principal value integrals and Hadamard finite-part integrals. The error estimation and convergence analysis for the corresponding method is also given. The new scheme based on numerical divided difference is of great accuracy and avoid the cancellation caused by the singular point $\xi$ effectively. Furthermore, the cycle index of the symmetric group allows evaluating the quadrature more efficiently.

**Acknowledgements**

The author would like to thank Prof. Xinghua Wang (Zhejiang University, PRC) for his helpful suggestions and constructive criticisms which greatly help completing the original manuscript.
Figure 5: the absolute errors of the approximations to $I_1(p = 0, m = 7, n = 8)$ for different singularities $\xi$.

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