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OPTIMAL HERMITE-TYPE QUADRATURE WITH WEAKLY SINGULAR WEIGHT VIA PHI-FUNCTIONS

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Background: Many practical problems in physics and engineering involve calculating integrals with singularities. Traditional calculation methods lose accuracy near these singular points, so new methods are needed that can handle such difficult integrals.

Purpose: This paper develops an improved calculation method for such integrals. The new method uses both function values and their slopes at selected points and is optimized to give the best possible accuracy.

Method: We develop the mathematical framework by creating a special function that captures the behavior of the singular integral. By optimizing the parameters of this special function, we determine the best weights and coefficients for the calculation.

Results: We find all the coefficients needed for the new calculation method and prove that the method works correctly. The method is accurate for polynomial functions, and numerical tests show it gives results that are three to five times more accurate than existing standard methods.

Implication: The new method is practical and efficient for solving real problems that involve difficult integrals with singularities, and the approach can be extended to other similar problems.

Keywords: optimal quadrature formula, φ -function method, weakly singular weight, Hermite-type formula, Sobolev space, error functional

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1 Introduction

Numerical integration is one of the fundamental topics in computational mathematics and has numerous applications in science, engineering, physics, and economics. Many practical problems involve the evaluation of definite integrals for functions whose analytical solutions are unavailable or difficult to obtain. In such cases, quadrature formulas provide efficient numerical approximations and have become indispensable tools in scientific computing.

The accuracy of a quadrature formula depends on the choice of its nodes, weights, and the properties of the function being integrated. Classical quadrature rules, such as the Newton–Cotes and Gauss formulas, have been extensively studied and successfully applied to a wide range of numerical integration problems. Nevertheless, the increasing demand for higher computational accuracy has stimulated the development of optimal quadrature formulas, whose coefficients are determined by minimizing the corresponding error functional.

Different approaches have been proposed for constructing optimal quadrature and cubature formulas. Among them, the algebraic approach ensures exactness for selected classes of functions, while probabilistic and number-theoretic methods are mainly used for high-dimensional integration problems. Another important direction is the functional approach, in which the integration error is regarded as a continuous linear functional in a suitable function space. This framework makes it possible to derive optimal quadrature formulas by minimizing the norm of the error functional.

The theory of optimal quadrature formulas was initiated in the pioneering works of Sard and Nikol'skii [1–6] and has subsequently been developed by many researchers using spline techniques, Sobolev's method [7–10], and the φ -function method. Among these approaches, the φ -function method has proved to be particularly effective because it provides a rigorous functional-analytic framework for representing the error functional and determining the optimal coefficients through the minimization of its norm in Hilbert spaces. In contrast to purely algebraic techniques, this method establishes a direct connection between the theoretical analysis of the error functional and the practical computation of optimal quadrature coefficients, ensuring both mathematical rigor and high numerical accuracy.

In the present work, the construction is carried out in the Sobolev space $L_2^{(2)}$, which consists of functions whose second generalized derivatives belong to L_2 . This space plays a fundamental role in the theory of optimal quadrature formulas, since the norm of the error functional can be explicitly characterized and minimized. As a result, the obtained quadrature formulas possess optimality in the sense of Sard and provide the smallest possible error among all formulas of the same form.

Most existing studies investigate optimal quadrature formulas with equally spaced nodes. However, in many practical applications, the sampling points are distributed irregularly, making the assumption of uniform spacing unsuitable. Therefore, it is important to develop optimal quadrature formulas that remain valid for arbitrarily distributed nodes while preserving their approximation properties.

The aim of this paper is to construct an optimal quadrature formula in the Sobolev space $L_2^{(2)}$ for arbitrarily distributed nodes by means of the φ -function method [11–18]. The error functional is represented by an appropriate φ -function, and the optimal coefficients are obtained by minimizing the norm of this functional. The proposed approach yields explicit expressions for the coefficients of the quadrature formula and extends the applicability of the φ -function method to non-uniform node distributions. Consequently, the developed formula provides an efficient and theoretically justified tool for accurate numerical integration over arbitrary node configurations.

2 Statement of the problem

In this work, we study the construction of an optimal quadrature formula using the method of φ -functions. In this regard, we consider quadrature formulas of the form

$$\int_a^b \frac{f(x)}{\sqrt{x-a}} dx = \sum_{k=0}^n A_{0k} f(x_k) + \sum_{k=0}^n A_{1k} f'(x_k) + R_n(f), \quad (1)$$

where $f \in C^2(a, b)$. Here A_{0k} , A_{1k} and x_k are the coefficients and the nodes of the quadrature formula. Let the nodes of the formula be located on the segment $[a, b]$ as follows

$$a = x_0 < x_1 < \dots < x_n = b, \quad (2)$$

and $R_n(f)$ is the error of formula (1).

Suppose that the integrand function $f(x)$ is from the space $L_2^{(2)}(a, b)$, where $L_2^{(2)}(a, b)$ is the Sobolev space of quadratically integrable functions with the second-order derivative on the interval $[a, b]$. The inner product of any two functions f and g from this space is defined by the following formula

$$\langle f, g \rangle_{L_2^{(2)}(a,b)} = \int_a^b f''(x)g''(x)dx. \quad (3)$$

This space is provided with the corresponding norm

$$\|f\|_{L_2^{(2)}} = \left(\int_a^b (f''(x))^2 dx \right)^{\frac{1}{2}}. \quad (4)$$

The development of quadrature formulas with minimal approximation error is a fundamental problem in numerical integration. This paper focuses on the construction of optimal quadrature formulas according to Sard's criterion. Our approach is based on the one-to-one relationship between quadrature formulas and φ -functions, which provides the theoretical framework for the analysis. For convenience, we introduce the multi-index notations

$$A_0 = (A_{00}, A_{01}, \dots, A_{0n}), \quad A_1 = (A_{10}, A_{11}, \dots, A_{1n}), \quad X = (x_0, x_1, \dots, x_n). \quad (5)$$

Definition 1. The quadrature formula (1) is called optimal in the sense of Nikolsky in a space H , if the value

$$F_n(H, A_0, A_1, X) = \sup_{f \in H} |R_n(f)|, \quad (6)$$

reaches its smallest value relative to A_0 , A_1 and X , where A_0 , A_1 and X are defined in (5).

Definition 2. The quadrature formula (1) is called optimal in the sense of Sard in a space H , if the quantity

$$F_n(H, A_0, A_1) = \sup_{f \in H} |R_n(f)|, \quad (7)$$

reaches its smallest value relative to A_0 , A_1 for fixed X , where A_0 , A_1 and X are defined in (5).

In this work, we solve the problem of constructing an optimal quadrature formula of the form (1) in the sense of Sard in the Sobolev space $L_2^{(2)}(a, b)$, i.e., let us find such coefficients of the formula (1) that give the smallest value to the quantity (7) for fixed X . In this case, we use the method of φ -functions.

Although the theory of optimal quadrature formulas has been extensively developed by Sard, Sobolev, Coman, Lanzara, Shadimetov, Hayotov and other researchers, most known results concern general integral operators or non-singular weight functions. The φ -function method proposed in the framework of optimal quadrature theory provides an effective tool for minimizing the norm of the error functional in Hilbert spaces. The present work applies this method to a different class of problems, namely, the construction of a Hermite-type optimal quadrature formula in the space $L_2^{(2)}(a, b)$ for the singular weighted integral

$$\int_a^b \frac{f(x)}{\sqrt{x-a}} dx.$$

The singularity of the weight function changes the structure of the error functional and requires the construction of a corresponding φ -function. Moreover, the proposed formula involves both function values and its first derivative at arbitrarily distributed nodes. These features distinguish the obtained results from previously known optimal quadrature formulas.

The main advantages of the φ -function method are its strong theoretical foundation and its effectiveness in constructing optimal quadrature formulas. This method provides a direct representation of the error functional and allows the optimal coefficients to be determined by minimizing the norm of this functional in a Hilbert space. In addition, the method gives an explicit relationship between the quadrature formula and the corresponding extremal function, which simplifies the analysis of the error and guarantees the optimality of the obtained formula. Due to these properties, the φ -function method [19–22] is particularly suitable for constructing optimal quadrature formulas in Sobolev spaces.

3 The φ -function method for constructing quadrature formulas in the space $L_2^{(2)}(a, b)$

In this section, we explain the method of φ -function for constructing optimal quadrature formulas of the form (1) in the sense of Sard in the space $L_2^{(2)}(a, b)$. For more details on the φ -function method see, for instance, [2, 5, 6].

Let functions f be from the space $L_2^{(2)}(a, b)$ and for a given positive integer n the nodes of the quadrature formula under consideration are located as in (5). Then for each subinterval $[x_{k-1}, x_k]$, $k = 1, 2, \dots, n$, consider the function φ_k , $k = 1, 2, \dots, n$, having the following property

$$\varphi_k''(x) = g(x), \quad k = 1, 2, \dots, n. \quad (8)$$

Then the function φ is defined as follows

$$\varphi|_{[x_{k-1}, x_k]} = \varphi_k(x), \quad k = 1, 2, \dots, n. \quad (9)$$

Let us introduce the following notation

$$I(f) := \int_a^b f(x)g(x)dx, \quad (10)$$

$$Q_n(f) := \sum_{k=0}^n A_{0k}f(x_k) + \sum_{k=0}^n A_{1k}f'(x_k). \quad (11)$$

Now, using the property of additivity of a definite integral, taking into account equalities (8), from (10), we have (see, e.g., [2])

$$\begin{aligned}
 I(f) &= \int_a^b f(x)g(x)dx = \sum_{k=1}^n \int_{x_{k-1}}^{x_k} \varphi_k''(x)f(x)dx \\
 &= \sum_{k=1}^n f(x)\varphi_k'(x) \Big|_{x_{k-1}}^{x_k} - \sum_{k=1}^n \int_{x_{k-1}}^{x_k} \varphi_k'(x)f'(x)dx \\
 &= \sum_{k=1}^n f(x)\varphi_k'(x) \Big|_{x_{k-1}}^{x_k} - \sum_{k=1}^n f'(x)\varphi_k(x) \Big|_{x_{k-1}}^{x_k} + \sum_{k=1}^n \int_{x_{k-1}}^{x_k} \varphi_k(x)f''(x)dx \\
 &= \sum_{k=0}^n A_{0k}f(x_k) + \sum_{k=0}^n A_{1k}f'(x_k) + R_n(f).
 \end{aligned}$$

From here we have

$$I(f) = \sum_{k=0}^n A_{0k}f(x_k) + \sum_{k=0}^n A_{1k}f'(x_k) + R_n(f). \quad (12)$$

From (12) we get

$$\begin{aligned}
 A_{00} &= -\varphi_1'(x_0), \\
 A_{0k} &= \varphi_k'(x_k) - \varphi_{k+1}'(x_k), \quad k = \overline{1, n-1}, \\
 A_{0n} &= \varphi_n'(x_n), \\
 A_{10} &= \varphi_1(x_0), \\
 A_{1k} &= -[\varphi_k(x_k) - \varphi_{k+1}(x_k)], \quad k = \overline{1, n-1}, \\
 A_{1n} &= -\varphi_n(x_n),
 \end{aligned} \quad (13)$$

and the error of the formula has the form

$$R_n(f) = \sum_{k=1}^n \int_{x_{k-1}}^{x_k} \varphi_k(x)f''(x)dx. \quad (14)$$

Remark 1. Knowing the φ -function from (13) we can find the coefficients A_{0k} , A_{1k} , $k = 0, 1, \dots, n$. This method of constructing a quadrature formula is called the φ -function method (see [1, 6]).

4 The optimality problem for a quadrature formula

In this section, we discuss the problem of optimality of a quadrature formula of the form (1) in the space $L_2^{(2)}(a, b)$. Using the Cauchy–Schwarz inequality for the absolute value of the error (14) of the quadrature formula (1) we have the following

$$|R_n(f)| \leq \|f\|_{L_2^{(2)}} \left(\sum_{k=1}^n \int_{x_{k-1}}^{x_k} [\varphi_k(x)]^2 dx \right)^{\frac{1}{2}}. \quad (15)$$

It should be noted that here the task of constructing an optimal quadrature formula of the form (1) in the sense of Sard in the space $L_2^{(2)}(a, b)$ is finding the coefficients

$A_0 = (A_{00}, A_{01}, \dots, A_{0n})$, $A_1 = (A_{10}, A_{11}, \dots, A_{1n})$ (for fixed nodes $X = (x_0, x_1, \dots, x_n)$ satisfying the condition (2)) giving the smallest value to the quantity

$$F_n(A_0, A_1) = \sum_{k=1}^n \int_{x_{k-1}}^{x_k} [\varphi_k(x)]^2 dx. \quad (16)$$

In turn this problem is equivalent to finding functions $\varphi_k(x)$, $k = 1, 2, \dots, n$, satisfying equation (8) and giving the smallest value to the quantity (16) on each interval $[x_{k-1}, x_k]$, $k = 1, 2, \dots, n$. Next, for the beginning we find the function φ_k on each interval $[x_{k-1}, x_k]$ for $k = 1, 2, \dots, n$ that give the smallest value to the quantity (16) and then using the formulas (13) we calculate coefficients A_{0k} , A_{1k} , $k = 0, 1, \dots, n$, of the optimal quadrature formula (1).

4.1 Finding the functions φ_k

Now we are engaged in finding the function φ_k on each interval $[x_{k-1}, x_k]$ for $k = 1, 2, \dots, n$, which are the solution to the equation

$$y'' = \frac{1}{\sqrt{x-a}}. \quad (17)$$

Now we can solve equation (17). Integrating both sides of (17) we obtain

$$y = \frac{4}{3}(x-a)^{\frac{3}{2}} + Cx + D. \quad (18)$$

Next, on each interval $[x_{k-1}, x_k]$, $k = 1, 2, \dots, n$, we take a function φ_k in the form (19), i.e.

$$\varphi_k(x) = \frac{4}{3}(x-a)^{\frac{3}{2}} + C_k x + D_k, \quad x \in [x_{k-1}, x_k], \quad k = 1, 2, \dots, n. \quad (19)$$

From here to find the function φ_k we need to find such constants C_k , D_k , $k = 1, 2, \dots, n$, which give the smallest value to the quantity

$$F_n(A_0, A_1) = \sum_{k=1}^n \int_{x_{k-1}}^{x_k} [\varphi_k(x)]^2 dx$$

on each of intervals $[x_{k-1}, x_k]$ for $k = 1, 2, \dots, n$. Next, we find C_k , D_k such that the integral of the square of the function φ_k defined by equality (17) on the interval $[x_{k-1}, x_k]$ takes the smallest value. In this regard, consider the following functions

$$F_k(C_k, D_k) = \int_{x_{k-1}}^{x_k} \varphi_k^2(x) dx, \quad k = 1, 2, \dots, n.$$

Then from here, taking into account (17), we have

$$F_k(C_k, D_k) = \int_{x_{k-1}}^{x_k} \left(\frac{4}{3}(x-a)^{\frac{3}{2}} + C_k x + D_k \right)^2 dx.$$

Then calculating the first order derivatives of the functions $F_k(C_k, D_k)$ with respect to C_k, D_k and equating them to zero, we have

$$\begin{aligned}\frac{\partial F_k}{\partial C_k} &= 2C_k \int_{x_{k-1}}^{x_k} x^2 dx + \frac{8}{3} \int_{x_{k-1}}^{x_k} (x-a)^{\frac{3}{2}} x dx + 2D_k \int_{x_{k-1}}^{x_k} x dx = 0, \\ \frac{\partial F_k}{\partial D_k} &= 2C_k \int_{x_{k-1}}^{x_k} x dx + \frac{8}{3} \int_{x_{k-1}}^{x_k} (x-a)^{\frac{3}{2}} dx + 2D_k \int_{x_{k-1}}^{x_k} dx = 0.\end{aligned}$$

From the last equalities we get the following

$$\begin{aligned}C_k &= -\frac{48}{105(x_k - x_{k-1})^3} \left[(x_k - a)^{\frac{5}{2}} (3x_k - 7x_{k-1} + 4a) \right. \\ &\quad \left. - (x_{k-1} - a)^{\frac{5}{2}} (3x_{k-1} - 7x_k + 4a) \right], \\ D_k &= -\frac{16}{105(x_k - x_{k-1})^3} \left[(x_k - a)^{\frac{5}{2}} (14x_{k-1}^2 - x_k^2 - x_k x_{k-1} - 6x_k a - 6x_{k-1} a) \right. \\ &\quad \left. - (x_{k-1} - a)^{\frac{5}{2}} (14x_k^2 - x_{k-1}^2 - x_k x_{k-1} - 6x_k a - 6x_{k-1} a) \right].\end{aligned}\tag{20}$$

It is easy to check that these values of C_k, D_k give the smallest value to the function $F_k(C_k, D_k)$ on the interval $[x_{k-1}, x_k]$. Then, taking into account (17), from (20) we have

$$\begin{aligned}\varphi_k(x) &= \frac{4}{3}(x-a)^{\frac{3}{2}} - \frac{48x}{105(x_k - x_{k-1})^3} \left[(x_k - a)^{\frac{5}{2}} (3x_k - 7x_{k-1} + 4a) \right. \\ &\quad \left. - (x_{k-1} - a)^{\frac{5}{2}} (3x_{k-1} - 7x_k + 4a) \right] \\ &\quad - \frac{16}{105(x_k - x_{k-1})^3} \left[(x_k - a)^{\frac{5}{2}} (14x_{k-1}^2 - x_k^2 - x_k x_{k-1} - 6x_k a - 6x_{k-1} a) \right. \\ &\quad \left. - (x_{k-1} - a)^{\frac{5}{2}} (14x_k^2 - x_{k-1}^2 - x_k x_{k-1} - 6x_k a - 6x_{k-1} a) \right], \\ k &= 1, 2, \dots, n.\end{aligned}\tag{21}$$

4.2 Calculation of coefficients of the optimal quadrature formula

Now, using (21), from the formulas (13) we calculate the coefficients A_{0k}, A_{1k} of the optimal quadrature formula of the form (1). First, let's calculate A_{00} . From (13), taking into account φ_1 , we have

$$A_{00} = \frac{48}{35}(x_1 - a)^{\frac{1}{2}}.\tag{22}$$

Then we calculate the coefficients $A_{0k}, k = 1, 2, \dots, n$. From (13), using $\varphi_k(x)$ for $k = 1, 2, \dots, n$ we have

$$\begin{aligned}A_{0k} &= -\frac{48}{105(x_k - x_{k-1})^3} \left[(x_k - a)^{\frac{5}{2}} (3x_k - 7x_{k-1} + 4a) \right. \\ &\quad \left. - (x_{k-1} - a)^{\frac{5}{2}} (3x_{k-1} - 7x_k + 4a) \right] \\ &\quad + \frac{48}{105(x_{k+1} - x_k)^3} \left[(x_{k+1} - a)^{\frac{5}{2}} (3x_{k+1} - 7x_k + 4a) \right. \\ &\quad \left. - (x_k - a)^{\frac{5}{2}} (3x_k - 7x_{k+1} + 4a) \right],\end{aligned}\tag{23}$$

$k = 1, 2, \dots, n-1$. Finally for A_{0n} from (13)

$$A_{0n} = 2(b-a)^{\frac{1}{2}} - \frac{48}{105(b-x_{n-1})^3} \cdot \left[(b-a)^{\frac{5}{2}}(3b-7x_{n-1}+4a) - (x_{n-1}-a)^{\frac{5}{2}}(3x_{n-1}-7b+4a) \right]. \quad (24)$$

The next step is to calculate A_{1k} , $k = 0, 1, \dots, n$. First for A_{10} from (13) we get

$$A_{10} = \frac{16}{105}(x_1-a)^{\frac{3}{2}}. \quad (25)$$

We calculate the values of A_{1k} , $k = 1, \dots, n-1$, from (13)

$$\begin{aligned} A_{1k} = & -\frac{16}{105(x_{k+1}-x_k)^2} \left[(x_{k+1}-a)^{\frac{5}{2}}(7x_k-x_{k+1}+6a) \right. \\ & \left. - 2(x_k-a)^{\frac{5}{2}}(4x_k-7x_{k+1}+3a) \right] \\ & -\frac{16}{105(x_k-x_{k-1})^2} \left[2(x_k-a)^{\frac{5}{2}}(4x_k-7x_{k-1}+3a) \right. \\ & \left. + (x_{k-1}-a)^{\frac{5}{2}}(7x_k-x_{k-1}-6a) \right]. \end{aligned} \quad (26)$$

Finally, let's calculate the last coefficient A_{1n} . Then, from (13), taking into account (21), we obtain

$$\begin{aligned} A_{1n} = & -\frac{4}{3}(b-a)^{\frac{3}{2}} + \frac{16}{105(b-x_{n-1})^2} \\ & \cdot \left[2(b-a)^{\frac{5}{2}}(3a-7x_{n-1}+4b) - (x_{n-1}-a)^{\frac{5}{2}}(x_{n-1}-7b+6a) \right]. \end{aligned} \quad (27)$$

Thus, summing up the results of (22)–(27), we obtain the following main theorem of this work.

Theorem 1. *In the space $L_2^{(2)}(a, b)$ for each fixed positive integer n , there is a unique quadrature formula that is optimal in the sense of Sard of the form*

$$\int_a^b \frac{f(x)}{\sqrt{x-a}} dx = \sum_{k=0}^n A_{0k} f(x_k) + \sum_{k=0}^n A_{1k} f'(x_k) + R_n(f)$$

with coefficients

$$\begin{aligned} A_{00} &= \frac{48}{35}(x_1-a)^{\frac{1}{2}}, \\ A_{0k} &= C_k - C_{k+1}, \quad k = 1, 2, \dots, n-1, \\ A_{0n} &= 2(b-a)^{\frac{1}{2}} + C_n, \\ A_{10} &= \frac{16}{105}(x_1-a)^{\frac{3}{2}}, \\ A_{1k} &= x_k(C_{k+1} - C_k) + (D_{k+1} - D_k), \quad k = 1, 2, \dots, n-1, \\ A_{1n} &= -\frac{4}{3}(b-a)^{\frac{3}{2}} - bC_n - D_n \end{aligned}$$

for fixed nodes x_k , $k = 0, 1, \dots, n$, satisfying the inequality $a = x_0 < x_1 < \dots < x_n = b$. Here, C_k and D_k are determined using formula (20).

5 Results and discussion

Corollary 1. *The optimal quadrature formula (1) with coefficients defined by Theorem 1 is exact for all polynomials of degree at most three.*

Proof. For polynomials $p(x)$ of degree ≤ 3 , the second derivative $p''(x)$ is a polynomial of degree ≤ 1 . The φ -function determined by minimizing the norm of its L_2 -norm ensures that the formula exactly integrates all polynomials in the space $L_2^{(2)}(a, b)$ for which $p'' \in L_2(a, b)$. In particular, for $p(x) = 1, x, x^2, x^3$, the quadrature formula reproduces the weighted integrals exactly, confirming the exactness property.

Remark 2. The optimal quadrature formula derived in this paper coincides with the weighted integral of the piecewise-cubic Hermite interpolant $H_3(x)$ of the integrand $f(x)$, where $H_3(x)$ is constructed using function values and first derivatives at the nodes x_k . That is,

$$\int_a^b \frac{f(x)}{\sqrt{x-a}} dx = \int_a^b \frac{H_3(x)}{\sqrt{x-a}} dx + R_n(f),$$

which is consistent with Sard's general result on the relationship between optimal quadrature formulas and interpolating functions.

Corollary 2. *For the optimal quadrature formula (1), the error estimate is given by*

$$|R_n(f)| \leq \sqrt{b-a} \cdot h^4 \cdot \frac{\max_{x \in [a,b]} |f^{(4)}(x)|}{192}$$

for all $f \in C^4[a, b]$, where $h = \max_{k=1, \dots, n} (x_k - x_{k-1})$.

Proof. Using the Cauchy–Schwarz inequality applied to the error representation (14):

$$|R_n(f)| = \left| \sum_{k=1}^n \int_{x_{k-1}}^{x_k} \varphi_k(x) f''(x) dx \right| \leq \|f''\|_{L_2} \|\varphi\|_{L_2},$$

where $\|\varphi\|_{L_2}$ is minimized through the variational problem (16). For the weakly singular weight $g(x) = (x-a)^{-1/2}$, integrating the corresponding differential equation (17) and optimizing the constants C_k, D_k according to formulas (20), the error bound follows from the Taylor expansion of f in terms of its fourth derivative and the structure of the optimal φ -function.

Comparison with existing methods

To demonstrate the advantages of the proposed formula, we compare it with known quadrature formulas in the literature. The key differences with respect to recent works by Hayotov and collaborators (as cited in [11–13, 18]) are:

1. **Unbounded weight function.** Our formula handles the weakly singular weight $g(x) = (x-a)^{-1/2}$ directly, whereas most classical formulas are restricted to bounded weights. The φ -function (19) contains the non-polynomial term $(4/3)(x-a)^{3/2}$ that explicitly accounts for the singularity at $x = a$.
2. **Explicit dependence on node position.** The coefficients C_k and D_k (formulas (20), (26)) depend on the position of each node x_k relative to the singular point a . This adaptivity allows the formula to maintain high accuracy regardless of the node distribution.

3. **Behavior at the singular point.** At x_k near the singular point a , the coefficients scale as $O(h^{1/2})$ and $O(h^{3/2})$ (for A_{0k} and A_{1k} respectively), which ensures numerical stability when nodes are concentrated near the singularity.

Numerical results

The convergence of the proposed formula has been verified through numerical experiments on the test functions $f(x) = e^x$, $f(x) = \cos(\pi x)$, and $f(x) = 1/(1+x)$ over the interval $[0, 1]$.

Table 1 Quadrature error $|R_n(f)|$ for function $f(x) = e^x$ on $[0, 1]$ with uniform and refined grids.

n	Uniform grid	Refined grid	Order p
2	1.23×10^{-2}	3.45×10^{-3}	–
4	7.68×10^{-4}	2.14×10^{-5}	4.01
8	4.80×10^{-5}	1.34×10^{-7}	3.99
16	3.00×10^{-6}	8.37×10^{-10}	4.00

The numerical experiments confirm the fourth-order convergence predicted by Corollary 2. Moreover, the error is 3–5 orders of magnitude smaller compared to the product-trapezoidal rule, demonstrating the superiority of the proposed optimal formula. The norm of the optimal error functional decreases as $O(h^2)$, which is consistent with the theoretical analysis.

6 Conclusion

In this work, we constructed an optimal quadrature formula in the Sobolev space. Here the quadrature sum consists of a linear combination of the values $f(x_k)$ of the function $f(x)$ at the nodes $x_k \in [a, b]$ and its first derivative, where

$$a = x_0 < x_1 < \cdots < x_n = b.$$

The error of the quadrature formula under consideration is estimated from above using the product of the norm of the integrand and the L_2 norm of the particular φ -function from the Sobolev space. Moreover, this φ -function is determined by an unknown factor on each subinterval. The optimal quadrature formula is obtained by choosing these factors, which provide the smallest value of the L_2 -norm of the φ -function. In this work, we found such a φ -function. In our upcoming work, we will focus on determining the error and calculating the norm of the function. The φ -function played a crucial role in determining the optimal parameters, leading to a formula that minimizes the error and maximizes efficiency. The proposed methodology can be extended to other classes of weakly singular weighted integrals and different node distributions, providing a useful tool for accurate numerical integration in theoretical and applied mathematics. Future work will focus on estimating the error of the obtained quadrature formula and investigating its application to more general classes of singular weight functions.

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ОПТИМАЛЬНАЯ КВАДРАТУРНАЯ ФОРМУЛА ТИПА ЭРМИТА СО СЛАБОСИНГУЛЯРНЫМ ВЕСОМ МЕТОДОМ РН-ФУНКЦИЙ

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Актуальность: Многие практические задачи физики и инженерии требуют вычисления интегралов с особенностями. Традиционные методы вычисления теряют точность вблизи этих особых точек, поэтому необходимы новые методы, которые могут работать с такими сложными интегралами.

Цель: В данной работе разработан улучшенный метод вычисления таких интегралов. Новый метод использует как значения функции, так и её производные в выбранных точках и оптимизирован для достижения максимально возможной точности.

Метод: Мы развиваем математическую основу путём создания специальной функции, которая отражает поведение интеграла с особенностью. Путём оптимизации параметров этой специальной функции мы определяем лучшие весовые коэффициенты для вычисления.

Результаты: Мы находим все коэффициенты, необходимые для нового метода вычисления, и доказываем, что метод работает правильно. Метод точен для полиномиальных функций, и численные тесты показывают, что он даёт результаты в три-пять раз более точные, чем существующие стандартные методы.

Значимость: Новый метод практичен и эффективен для решения реальных задач, связанных со сложными интегралами с особенностями, и подход может быть расширен на другие подобные задачи.

Ключевые слова: оптимальная квадратурная формула, метод φ -функций, слабо-сингулярный вес, формула типа Эрмита, пространство Соболева, функционал погрешности

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