

On Optimality and Error Estimation of a Quadrature Formula With Derivative That Is Exact for Trigonometric Functions

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Abstract. In this paper, we investigate the determination of coefficients for an optimal quadrature formula involving derivatives by applying the φ -function technique. The φ -function approach enables the development of optimal quadrature rules for approximating definite integrals. In this work when the nodes are arbitrarily fixed, the conditions for the optimality of the quadrature rule are examined, and the approach for identifying the elements of the formula is discussed. Explicit expressions for the coefficients of the optimal quadrature formula are derived. Specifically, when the nodes are equally distributed, an Euler-Maclaurin type optimal quadrature rule is achieved.

1. INTRODUCTION

The *definite integral* is a fundamental concept in mathematical analysis and has wide-ranging applications. In particular, it is used to compute the area under a curve or the surface area over a region bounded by the graph of a function. However, in many cases, obtaining the antiderivative (also called the primitive function) of the integrand is either very difficult or impossible. Therefore, a variety of *numerical integration methods*, also known as *quadrature formulas*, have been developed to approximate definite integrals.

It is well known from classical analysis that when the antiderivative of the integrand is available, the integral can be evaluated using the Newton–Leibniz formula. In cases where this is not feasible, one must approximate the integral using numerical techniques. To address this, mathematicians have constructed many quadrature and cubature formulas [1, 4, 13, 16, 17, 21].

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In this study, we derive an *optimal quadrature formula* in the space $K_2^{(2,0)}$ using the φ -function method. This space is a Hilbert space and represents a particular case of function spaces frequently considered in numerical analysis. Several works such as [6, 8, 13] have studied this problem.

When the nodes of the quadrature formula are selected arbitrarily, methods such as the spline method, the φ -function method, and the Sobolev method can be employed to construct of optimal quadrature formulas by minimizing the norm of the associated error functional, often considering the distribution of the nodes.

Researchers including A. Ghizzetti and A. Ossicini [23], F. Lanzara [16], and T. Catinas and G. Coman [2] have developed optimal quadrature formulas using these methods. In this paper, we investigate the problem of constructing an optimal quadrature formula in the sense of Sard. The coefficients of the resulting formula are computed using the corresponding φ -function, ensuring optimality.

The obtained quadrature formula is exact for the functions $\sin(x)$ and $\cos(x)$ [6].

In this work, we also extend the results of [10] by considering a family of quadrature formulas and providing a sharp upper bound estimate for the remainder term $R_n(f)$

$$\int_a^b f(x) dx = \sum_{k=0}^n A_{0k} f(x_k) + \sum_{k=0}^n A_{1k} f'(x_k) + R_n(f), \quad (1.1)$$

where A_{0k} , A_{1k} , and x_k are the coefficients and nodes, respectively.

Let the nodes be distributed over the interval $[a, b]$ in the following manner,

$$a = x_0 < x_1 < \dots < x_n = b. \quad (1.2)$$

Let us suppose that the function f , appearing under the integral, belongs to the space $K_2^{(2,0)}$, where $K_2^{(2,0)} := \{f : [a, b] \rightarrow \mathbb{R} | f' - \text{absolute continuous and } f'' \in L_2(a, b)\}$. In this space, the inner product of two arbitrary functions f and g is defined as

$$\langle f, g \rangle_{K_2^{(2,0)}} = \int_a^b (f''(x) + f(x))(g''(x) + g(x)) dx.$$

The associated norm in this space is given by the expression

$$\|f\|_{K_2^{(2,0)}} = \left(\int_a^b (f''(x) + f(x))^2 dx \right)^{1/2}.$$

We aim to develop a quadrature rule of the form (1.1) that yields the minimal error when approximating functions in the space $K_2^{(2,0)}$. For simplicity, we adopt the following notations:

$$A_0 = (A_{00}, A_{01}, \dots, A_{0n}), \quad A_1 = (A_{10}, A_{11}, \dots, A_{1n}) \quad \text{and} \quad X = (x_0, x_1, \dots, x_n). \quad (1.3)$$

Below we provide the definitions of optimality and quadrature rules as given in ([3, 6, 18]).

Definition 1.1. The quadrature formula of the form (1.1) is called optimal in the Nikolysky sense in the space $K_2^{(2,0)}$ if the quantity

$$F_n(K_2^{(2,0)}, A_0, A_1, X) = \sup_{f \in K_2^{(2,0)}} |R_n(f)|$$

reaches its smallest value with respect to A_0, A_1 and X , and A_0, A_1 and X are defined by equality (1.3).

Definition 1.2. The quadrature formula (1.1) is called optimal in the sense of Sard in the space $K_2^{(2,0)}$ if the quantity

$$F_n(K_2^{(2,0)}, A_0, A_1) = \sup_{f \in K_2^{(2,0)}} |R_n(f)|$$

reaches its smallest value relative to A_0, A_1 for fixed X , where A_0, A_1 and X are given by (1.3).

In this paper we construct optimal quadrature formula of the form (1.1) in the sense of Sard in the Hilbert space $K_2^{(2,0)}$. The quadrature formula is exact for trigonometric functions $\sin(x)$ and $\cos(x)$. The rest of the work is organized as follows.

In section 2 we discuss the φ - function method for construction of quadrature formulas of the form (1.1) in the space $K_2^{(2,0)}$. In section 3, we consider the optimization of the quadrature formulas of the form (1.1). We get the explicite expressions of coefficients for the optimal formula. In particular, we get the Euler - Maclaurin type quadrature formula in the space $K_2^{(2,0)}$.

2. CONSTRUCTION OF QUADRATURE FORMULAS USING THE φ - FUNCTION METHOD IN $K_2^{(2,0)}$

Let the function f belong to the space $K_2^{(2,0)}$, and suppose that for a given natural number n , the nodes are arranged according to the distribution of the form (1.2). Then, for each subinterval $[x_{k-1}, x_k]$, where $(k = 1, 2, \dots, n)$, we examine the function φ_k , $k = 1, 2, \dots, n$ that satisfies the property

$$\varphi_k''(x) + \varphi_k(x) = 1, \quad k = 1, 2, \dots, n. \quad (2.1)$$

Then the function φ is defined as follows

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

Hence, the restriction of the function φ on the interval $[x_{k-1}, x_k]$ is given by φ_k .

We introduce the following notations:

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

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

Utilizing the properties of additivity and piecewise integration of definite integrals, and considering identity (2.1), we arrive at

$$I(f) = \int_a^b f(x) dx = \sum_{k=1}^n \int_{x_{k-1}}^{x_k} f(x) dx = \sum_{k=1}^n \int_{x_{k-1}}^{x_k} (\varphi_k''(x) + \varphi_k(x)) f(x) dx.$$

Then integrating by parts we have

$$\begin{aligned} I(f) &= \varphi_n'(x_n)f(x_n) + \sum_{k=1}^{n-1} \varphi_k'(x_k)f(x_k) - \varphi_1'(x_0)f(x_0) - \sum_{k=1}^{n-1} \varphi_{k+1}'(x_k)f(x_k) - \varphi_n(x_n)f'(x_n) \\ &\quad - \sum_{k=1}^{n-1} \varphi_k(x_k)f'(x_k) + \varphi_1(x_0)f'(x_0) + \sum_{k=1}^{n-1} \varphi_{k+1}(x_k)f'(x_k) + \sum_{k=1}^n \int_{x_{k-1}}^{x_k} (f''(x) + f(x)) \varphi_k(x) dx. \end{aligned}$$

From this we get the following:

$$\begin{aligned} I(f) &= -\varphi_1'(x_0) + \sum_{k=1}^{n-1} (\varphi_k'(x_k) - \varphi_{k+1}'(x_k))f(x_k) + \varphi_n'(x_n)f(x_n) \\ &\quad + \varphi_1(x_0)f'(x_0) - \sum_{k=1}^{n-1} (\varphi_k(x_k) - \varphi_{k+1}(x_k))f'(x_k) - \varphi_n(x_n)f'(x_n) + R_n(f) \\ &= \sum_{k=0}^n A_{0k}f(x_k) + \sum_{k=0}^n A_{1k}f'(x_k) + R_n(f) \end{aligned} \quad (2.2)$$

From equality (2.2) we get:

$$\begin{aligned} A_{00} &= -\varphi_1'(x_0), \\ A_{0k} &= \varphi_k'(x_k) - \varphi_{k+1}'(x_k), \quad k = 1, 2, \dots, n-1, \\ A_{0n} &= \varphi_n'(x_n), \\ A_{10} &= \varphi_1(x_0), \\ A_{1k} &= \varphi_{k+1}(x_k) - \varphi_k(x_k), \quad k = 1, 2, \dots, n-1, \\ A_{1n} &= -\varphi_n(x_n), \end{aligned} \quad (2.3)$$

and the error of the formula is as follows,

$$R_n(f) = \sum_{k=1}^n \int_{x_{k-1}}^{x_k} (f''(x) + f(x)) \varphi_k(x) dx = \int_a^b (f''(x) + f(x)) \varphi(x) dx. \quad (2.4)$$

We now proceed to solve the following nonhomogeneous linear differential equation of second order:

$$y'' + y = 1 \quad (2.5)$$

and obtain the general solution in the following form

$$y = C_1 \cos(x) + C_2 \sin(x) + 1. \quad (2.6)$$

Remark 2.1. Knowing the function φ , one can find the coefficients A_{0k} and A_{1k} , $k = 0, 1, \dots, n$ from equality (2.3). This method is called the φ function method of constructing a quadrature formula [23].

Remark 2.2. As can be seen from expression (2.4) above, the quadrature formula (1.1) is exact to the functions that are solutions of the equation

$$f''(x) + f(x) = 0. \quad (2.7)$$

In the following sections, we deal with finding the coefficients of the optimal quadrature formula (1.1) in the space $K_2^{(2,0)}$.

3. DERIVATION OF AN OPTIMAL QUADRATURE FORMULA

This section focuses on analyzing the optimality of the quadrature formula (1.1) in the space $K_2^{(2,0)}$. Then, using the Cauchy-Schwarz inequality, we estimate the absolute value of the error (2.4) of formula (1.1) is the following from:

$$|R_n(f)| \leq \|f'' + f\|_{L_2(a,b)} \cdot \left(\int_a^b \varphi^2(x) dx \right)^{1/2} = \|f\|_{K_2^{(2,0)}} \cdot \|\varphi\|_{L_2(a,b)}.$$

Now we consider the function $\varphi_k(x)$, $x \in [x_{k-1}, x_k]$, $k = 1, 2, \dots, n$ as a solution of this equation (2.5). Then based on (2.6) for φ_k , we have

$$\varphi_k(x) = C_1^{(k)} \cdot \cos x + C_2^{(k)} \cdot \sin x + 1,$$

where $C_1^{(k)}$, $C_2^{(k)}$, $k = 1, 2, \dots, n$, are arbitrary constants.

In summary, in order to determine the functions $\varphi_k(x)$, it is required to identify the unknowns $C_1^{(k)}$ and $C_2^{(k)}$, $k = 1, 2, \dots, n$. We determine $C_1^{(k)}$ and $C_2^{(k)}$ such that the integral of the square of the function φ_k attains its minimum value. Let's look at this function that is related to these,

$$\mathcal{F}_k(C_1^{(k)}, C_2^{(k)}) = \int_{x_{k-1}}^{x_k} (\varphi_k(x))^2 dx, \quad k = 1, 2, \dots, n.$$

Then, taking into account (2.7), we have the following.

$$\mathcal{F}_k(C_1^{(k)}, C_2^{(k)}) = \int_{x_{k-1}}^{x_k} (C_1^{(k)} \cos(x) + C_2^{(k)} \sin(x) + 1)^2 dx$$

$$\begin{aligned}
&= \int_{x_{k-1}}^{x_k} \left((C_1^{(k)})^2 \cos^2(x) + (C_2^{(k)})^2 \sin^2(x) + 1 + 2 \cdot C_1^{(k)} C_2^{(k)} \cos(x) \sin(x) \right. \\
&\quad \left. + 2 \cdot C_1^{(k)} \cos(x) + 2 \cdot C_2^{(k)} \sin(x) \right) dx, k = 1, 2, \dots, n.
\end{aligned}$$

We calculate the first particular derivatives of this function with respect to $C_1^{(k)}$ and $C_2^{(k)}$ and equating them to zero we have the following system of equations

$$\begin{cases} a_{11} \cdot C_1^{(k)} + a_{12} \cdot C_2^{(k)} = b_1, \\ a_{21} \cdot C_1^{(k)} + a_{22} \cdot C_2^{(k)} = b_2, \end{cases}$$

where

$$\begin{aligned}
a_{11} &= \int_{x_{k-1}}^{x_k} \cos^2(x) dx, \\
a_{12} &= a_{21} = \int_{x_{k-1}}^{x_k} \sin(x) \cos(x) dx, \\
a_{22} &= \int_{x_{k-1}}^{x_k} \sin^2(x) dx, \\
b_1 &= - \int_{x_{k-1}}^{x_k} \cos(x) dx, \\
b_2 &= - \int_{x_{k-1}}^{x_k} \sin(x) dx.
\end{aligned}$$

Taking into account that

$$\begin{aligned}
a_{11} &= \frac{1}{2} \left(x_k - x_{k-1} + \frac{1}{2} (\sin(2x_k) - \sin(2x_{k-1})) \right), \\
a_{12} &= a_{21} = -\frac{1}{4} (\cos(2x_k) - \cos(2x_{k-1})), \\
a_{22} &= \frac{1}{2} \left(x_k - x_{k-1} - \frac{1}{2} (\sin(2x_k) - \sin(2x_{k-1})) \right), \\
b_1 &= -(\sin(x_k) - \sin(x_{k-1})), \\
b_2 &= \cos(x_k) - \cos(x_{k-1})
\end{aligned}$$

we get

$$\begin{aligned}
C_1^{(k)} &= -\frac{4 \cdot \sin\left(\frac{x_k - x_{k-1}}{2}\right) \cdot \cos\left(\frac{x_k + x_{k-1}}{2}\right)}{x_k - x_{k-1} + \sin(x_k - x_{k-1})}, \\
C_2^{(k)} &= -\frac{4 \cdot \sin\left(\frac{x_k - x_{k-1}}{2}\right) \cdot \sin\left(\frac{x_k + x_{k-1}}{2}\right)}{x_k - x_{k-1} + \sin(x_k - x_{k-1})}.
\end{aligned} \tag{3.1}$$

Then using (3.1) from (2.7) we come

$$\begin{aligned}\varphi_k(x) &= -\frac{4 \sin\left(\frac{x_k - x_{k-1}}{2}\right) \cos\left(\frac{x_k + x_{k-1}}{2}\right)}{x_k - x_{k-1} + \sin(x_k - x_{k-1})} \cos x \\ &\quad - \frac{4 \sin\left(\frac{x_k - x_{k-1}}{2}\right) \sin\left(\frac{x_k + x_{k-1}}{2}\right)}{x_k - x_{k-1} + \sin(x_k - x_{k-1})} \sin x + 1, \quad k = 1, 2, \dots, n.\end{aligned}\quad (3.2)$$

For the first derivative of φ we have

$$\begin{aligned}\varphi'_k(x) &= \frac{4 \sin\left(\frac{x_k - x_{k-1}}{2}\right) \cos\left(\frac{x_k + x_{k-1}}{2}\right)}{x_k - x_{k-1} + \sin(x_k - x_{k-1})} \sin(x) \\ &\quad - \frac{4 \sin\left(\frac{x_k - x_{k-1}}{2}\right) \sin\left(\frac{x_k + x_{k-1}}{2}\right)}{x_k - x_{k-1} + \sin(x_k - x_{k-1})} \cos(x).\end{aligned}\quad (3.3)$$

Now we can calculate the coefficients $A_{0k}, A_{1k}, k = 1, 2, \dots, n$ based on (2.3) for the optimal quadrature formula of the form (1.1) in the space $K_2^{(2,0)}$. From (2.3), taking into account (3.2) and (3.3) we get

$$\begin{aligned}A_{00} &= \frac{2 \cdot (1 - \cos(x_1 - x_0))}{x_1 - x_0 + \sin(x_1 - x_0)}, \\ A_{0k} &= \frac{2 \cdot (1 - \cos(x_k - x_{k-1}))}{x_k - x_{k-1} + \sin(x_k - x_{k-1})} + \frac{2 \cdot (1 - \cos(x_{k+1} - x_k))}{x_{k+1} - x_k + \sin(x_{k+1} - x_k)}, \quad k = 1, 2, \dots, n-1, \\ A_{0n} &= \frac{2 \cdot (1 - \cos(x_n - x_{n-1}))}{x_n - x_{n-1} + \sin(x_n - x_{n-1})}, \\ A_{10} &= \frac{x_1 - x_0 - \sin(x_1 - x_0)}{x_1 - x_0 + \sin(x_1 - x_0)}, \\ A_{1k} &= \frac{2 \cdot \sin(x_k - x_{k-1}) \cdot (x_{k+1} - x_k) - 2 \cdot \sin(x_{k+1} - x_k) \cdot (x_k - x_{k-1})}{(x_{k+1} - x_k + \sin(x_{k+1} - x_k)) \cdot (x_k - x_{k-1} + \sin(x_k - x_{k-1}))}, \quad k = 1, 2, \dots, n-1, \\ A_{1n} &= \frac{\sin(x_n - x_{n-1}) - (x_n - x_{n-1})}{x_n - x_{n-1} + \sin(x_n - x_{n-1})}.\end{aligned}\quad (3.4)$$

Thus we have obtained the following main result of this work.

Theorem 3.1. *For fixed nodes $a = x_0 < x_1 < \dots < x_n = b$ there exists a unique optimal quadrature formula of the form*

$$\int_a^b f(x) dx \cong \sum_{k=0}^n A_{0k} f(x_k) + \sum_{k=0}^n A_{1k} f'(x_k), \quad (3.5)$$

in the sense of Sard in the space $K_2^{(2,0)}$ with coefficients (3.4). The formula is exact for trigonometric functions $\sin(x)$ and $\cos(x)$.

From Theorem 3.1 when the nodes are equally spaced we get the optimal quadrature formula of the Euler - Maclaurin type in the space $K_2^{(2,0)}$. That is the following holds.

Corollary 3.1. For equally distributed nodes $x_k = a + kh$, $k = 0, 1, \dots, n$, and $h = \frac{b-a}{n}$, there exists a unique optimal quadrature formula

$$\int_a^b f(x) dx \cong \sum_{k=1}^n A_{0k} f(a + kh) + A_{10} f'(a) + A_{1n} f'(b)$$

of the Euler - Maclaurin type, defined by a corresponding set of weights

$$A_{00} = \frac{2 \cdot (1 - \cos(h))}{h + \sin(h)},$$

$$A_{0k} = \frac{4 \cdot (1 - \cos(h))}{h + \sin(h)}, \quad k = 1, 2, \dots, n-1,$$

$$A_{0n} = \frac{2 \cdot (1 - \cos(h))}{h + \sin(h)},$$

$$A_{10} = \frac{h - \sin(h)}{h + \sin(h)},$$

$$A_{1k} = 0, \quad k = 1, 2, \dots, n-1,$$

$$A_{1n} = \frac{\sin(h) - h}{h + \sin(h)}.$$

4. A SHARP UPPER ESTIMATE OF THE QUADRATURE FORMULA ERROR

Now, substituting the obtained expressions for C_1 and C_2 , we derive the general form of the $\varphi_k(x)$ - function, where $k = 1, 2, \dots, n$,

$$\varphi_k(x) = 1 - \frac{4 \cdot \sin\left(\frac{x_k - x_{k-1}}{2}\right) \cdot \cos\left(x - \frac{x_k + x_{k-1}}{2}\right)}{x_k - x_{k-1} + \sin(x_k - x_{k-1})}. \quad (4.1)$$

Next, we evaluate the square of the $\varphi_k(x)$ -function and perform integration over the interval $[x_{k-1}, x_k]$

$$\int_{x_{k-1}}^{x_k} \varphi_k^2(x) dx = \int_{x_{k-1}}^{x_k} \left(\frac{4 \sin^2\left(\frac{x_k - x_{k-1}}{2}\right)}{x_k - x_{k-1} + \sin(x_k - x_{k-1})} \cos\left(x - \frac{x_k + x_{k-1}}{2}\right) - 1 \right)^2 dx$$

$$\begin{aligned}
&= \frac{16 \sin^2\left(\frac{x_k - x_{k-1}}{2}\right)}{\left(x_k - x_{k-1} + \sin(x_k - x_{k-1})\right)^2} \int_{x_{k-1}}^{x_k} \cos^2\left(x - \frac{x_k + x_{k-1}}{2}\right) dx \\
&\quad - \frac{8 \sin\left(\frac{x_k - x_{k-1}}{2}\right)}{x_k - x_{k-1} + \sin(x_k - x_{k-1})} \int_{x_{k-1}}^{x_k} \cos\left(x - \frac{x_k + x_{k-1}}{2}\right) dx + \int_{x_{k-1}}^{x_k} dx \\
&= \frac{8 \sin^2\left(\frac{x_k - x_{k-1}}{2}\right)}{\left(x_k - x_{k-1} + \sin(x_k - x_{k-1})\right)^2} \left(x + \frac{1}{2} \sin(2x - x_k - x_{k-1})\right) \Big|_{x_{k-1}}^{x_k} \\
&\quad - \frac{8 \sin\left(\frac{x_k - x_{k-1}}{2}\right)}{x_k - x_{k-1} + \sin(x_k - x_{k-1})} \sin\left(x - \frac{x_k + x_{k-1}}{2}\right) \Big|_{x_{k-1}}^{x_k} + (x_k - x_{k-1}) \\
&= (x_k - x_{k-1}) - \frac{4(1 - \cos(x_k - x_{k-1}))}{x_k - x_{k-1} + \sin(x_k - x_{k-1})}.
\end{aligned}$$

Hence,

$$\int_{x_{k-1}}^{x_k} \varphi_k^2(x) dx = x_k - x_{k-1} - \frac{4(1 - \cos(x_k - x_{k-1}))}{x_k - x_{k-1} + \sin(x_k - x_{k-1})}. \quad (4.2)$$

Next, we evaluate the norm of the function $\varphi(x)$:

$$\|\varphi\|_{L_2(a,b)}^2 = \sum_{k=1}^n \left[x_k - x_{k-1} - \frac{4(1 - \cos(x_k - x_{k-1}))}{x_k - x_{k-1} + \sin(x_k - x_{k-1})} \right]. \quad (4.3)$$

$$|R_n(f)| \leq \|f'' + f\|_{L_2(a,b)} \cdot \left(\int_a^b \varphi^2(x) dx \right)^{1/2} = \|f\|_{K_2^{(2,0)}} \cdot \|\varphi\|_{L_2(a,b)}$$

$$= \|f\|_{K_2^{(2,0)}} \cdot \sqrt{\sum_{k=1}^n \left[x_k - x_{k-1} - \frac{4(1 - \cos(x_k - x_{k-1}))}{x_k - x_{k-1} + \sin(x_k - x_{k-1})} \right]}.$$

For equally distributed (uniformly spaced) nodes, the following formula can be derived.

$$\|\varphi\|_{L_2(a,b)}^2 = \sum_{k=1}^n \left[h - \frac{4(1 - \cos(h))}{h + \sin(h)} \right] \quad (4.4)$$

$$\|\varphi\|_{L_2(a,b)}^2 = n \cdot \left(h - \frac{4(1 - \cos(h))}{h + \sin(h)} \right),$$

$$= \left(\frac{h^4}{720} + \frac{h^6}{15120} + O(h^8) \right) \cdot (b - a)$$

5. CONCLUSION

In this work, we developed an optimal quadrature formula in the Hilbert space $K_2^{(2,0)}$, consisting of absolutely continuous functions whose second derivatives are square-integrable on the interval $[a, b]$. The φ -function method was employed to determine the structure and coefficients of the formula, playing a key role in minimizing the integration error. The proposed quadrature formula is suitable for both theoretical investigations and practical applications in numerical analysis, particularly, where precise approximation of definite integrals is required. The method also provides a foundation for constructing more advanced formulas in extended function spaces, indicating promising directions for future research.

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