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# AN OPTIMAL QUADRATURE FORMULA WITH DERIVATIVES FOR ARBITRARILY FIXED NODES IN THE SOBOLEV SPACE

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The numerical computation of definite integrals plays a crucial role in various applied and theoretical disciplines. In many cases, exact analytical evaluation of integrals is infeasible due to the complexity of the integrand or the nature of the integration limits. Quadrature formulas provide an efficient approach for approximating definite integrals, relying on weighted sums of function values at selected nodes. Traditional quadrature formulas, such as those of Newton-Cotes, Gauss, aim to optimize accuracy by carefully choosing nodes and weights. However, optimal quadrature formulas can also be constructed in the sense of Sard, minimizing the error functional within a given function space. In this paper, we focus on constructing an optimal quadrature formula in the Sobolev space with arbitrarily fixed nodes. Unlike conventional approaches where coefficients are determined sequentially, we simultaneously optimize both function and derivative coefficients, improving overall accuracy and stability. The derivation employs the method of $\varphi$ - functions, which allows us to express the quadrature formula's coefficients explicitly and analyze its error properties. The obtained quadrature formula minimizes the error norm in the chosen function space, ensuring an improved approximation of definite integrals. Furthermore, when the nodes are equally spaced, our results generalize the well-known Euler-Maclaurin formula, demonstrating the effectiveness of our approach.

**Keywords:** quadrature formula, Sobolev space, optimal approximation, $\varphi$-function method, Euler-Maclaurin formula.

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## 1 Introduction

Many applied and theoretical problems often lead to the calculation of definite integrals. However, it is not always possible to compute these integrals analytically. In some cases, the function under the integral cannot be expressed in terms of elementary functions, or it may be given in tabular form. Additionally, the integration limits may be complex, or the function may have a special structure. In such situations, approximate methods for evaluating definite integrals become crucial.

The primary approach in approximating definite integrals involves computing function values at certain points and expressing the integral as a linear combination of these values. This method is widely used in mathematical modeling, engineering, physics, economics, and statistics. The development of numerical computation techniques has further enhanced the importance of such methods for efficiently calculating integrals.

One of the fundamental techniques for approximating definite integrals is the use of quadrature formulas. Quadrature formulas allow the evaluation of an integral using a finite number of function values at specific points. The construction of quadrature formulas and the evaluation of their error functionals are based on methods of functional analysis. Initial scientific contributions in this area were made by A. Sard, who demonstrated that the norm of the error functional can be minimized by adjusting the coefficients at fixed nodes. At the same time S. M. Nikolskii developed the theory of quadrature formulas, contributing significantly to the advancement of quadrature formula research.

It is noteworthy that different approaches, such as the spline method, the $\varphi$-function method, and the Sobolev method, have been employed to construct quadrature formulas. A. Sard proposed a method for deriving optimal quadrature formulas by minimizing the error functional based on the coefficients at fixed nodes. Contributions from L. F. Meyers, G. Coman, S. D. Silliman, P.Köhler , A. Ghizzetti, A. Ossicini, F. Lanzara, and T. Catinas have been instrumental in developing quadrature formulas using spline methods and the $\varphi$-function method.

In the Sobolev method, the construction of optimal quadrature formulas is based on determining the coefficients through a minimization process. S. L. Sobolev made significant contributions by generalizing previous research on spline methods and formulating quadrature structures within the $L_2^{(m)}$ space. Algorithms developed using the Sobolev method have been implemented in the scientific research of Kh. M. Shadimetov, A. R. Hayotov, and others.

Although the results presented in this paper are closely related to previous studies, our approach is specifically focused on jointly optimizing the coefficients of a function and its derivative at fixed nodes. This work aims to further refine the structure of quadrature formulas and optimize their coefficients, contributing to the ongoing research in numerical integration methods.

The works of T.Catinas and G.Coman [3], F.Lanzara [4], A.Ghizzetti and A.Ossicini [5] using the method of $\varphi$-functions, constructed optimal quadrature formulas in the $L_2^{(m)}$ space. In particular, in works [3] and [4] the coefficients in front of the function and its derivative were sequentially optimized.

Our approach fully accounts for the interdependence between the function and its derivatives during the integration process, leading to improved accuracy in the quadrature formula.

## 2 Problem statement

In this paper, we consider a quadrature formula of the form:

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

where $A_{0k}$, $A_{1k}$, and $x_k$ are the coefficients and the nodes of the quadrature formula. Let the nodes distributed in the interval $[a, b]$ as follows

$$a = x_0 < x_1 < x_2 < \cdots < x_n = b, \tag{2}$$

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

Assume that the integrand function $f$ is in the Sobolev space $L_2^{(2)}(a,b)$. In this space, the function itself, as well as its first and second-order derivatives belong to the class of functions that quadratically integrable on the interval $[a,b]$. The inner product of any two functions in this space is defined as follows:

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

The corresponding norm here has the form

$$\|f\|^2_{L_2^{(2)}} = \langle f,f\rangle = \int_a^b \left(f''(x)\right)^2 dx. \tag{4}$$

One of the important problems in the theory of quadrature formulas is the issue of optimality related to the error of the given formula. In this study, we consider the problem of optimality in the sense of Sard. Here, we use one-to-one correspondences between quadrature formulas and $\varphi$-functions.

For convenience, we introduce the following notations

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

**Definition 2.1.** The quadrature formula (1) is called optimal in the sense of Sard in the space $L_2^{(2)}(a,b)$ if the quantity

$$F_n\left(L_2^{(2)}(a,b), A_0, A_1\right) = \sup_{f\in L_2^{(2)}(a,b)} |R_n(f)|, \tag{6}$$

reaches its smallest value relative to $A_1$ and $A_2$ for fixed $X$, where $A_1, A_2$ and $X$ are defined in (5).

In this study, we focus on constructing an optimal quadrature formula of the form (1). Using the $\varphi$-functions method, we determine the coefficients $A_1$ and $A_2$ that minimize the expression (6).

In the next section, the working principle of the $\varphi$-functions method in the space $L_2^{(2)}$, as well as the relationship between the quadrature formula and $\varphi$-functions, is discussed. In Section 4, the optimality problem of the quadrature formula of the form (1) is examined, specifically by finding the $\varphi$-function that minimizes the error of the quadrature formula (1). Using the obtained $\varphi$-functions the analitic expressions of the coefficients $A_0$ and $A_1$ of the optimal quadrature formula (1) are calculated.

## 3 The $\varphi$-function method in $L_2^{(2)}(a,b)$ space

In this section, we explain the method of $\varphi$-function for constructing optimal quadrature formulas of the form (1) in the sense of Sard in the space $L_2^{(2)}(a,b)$. Let $f$ be from $L_2^{(2)}(a,b)$ space and the nodes be distributed as in (2) for the given natural number $n$. Then for each interval $[x_{k-1}, x_k]$ $\quad (k = 1,2,\dots,n)$ consider the functions $\varphi_k$, $k = 1,2,\dots,n$ having the following property

$$\varphi_k''(x) = 1, \quad k = 1,2,\dots,n. \tag{7}$$

Then a $\varphi$-function is defined as

$$\varphi\Big|_{[x_{k-1},x_k]} = \varphi_k, \quad k = 1,2,\dots,n. \tag{8}$$

Thus, in the interval $[x_{k-1}, x_k]$, the contraction of the $\varphi$-function is equal to $\varphi_k$.

Then we have the following relations between the $\varphi$ function and coefficients of the formula (1).

**Lemma 3.1.** *The coefficients $A_0, A_1$ of the quadrature formula in the form of (1) and the error functional are expressed through the $\varphi_k$-functions as follows*

$$\begin{gathered} A_{00} = -\varphi_1'(x_0), \\ A_{0k} = \varphi_k'(x_k) - \varphi_{k+1}'(x_k), \quad k = 1, 2, \ldots, n-1, \\ A_{0n} = \varphi_n'(x_n), \\ A_{10} = \varphi_1(x_0), \\ A_{1k} = \varphi_{k+1}(x_k) - \varphi_k(x_k), \quad k = 1, 2, \ldots, n-1, \\ A_{1n} = -\varphi_n(x_n). \end{gathered} \tag{9}$$

*and the error of the formula has the form*

$$R_n(f) = \sum_{k=1}^{n} \int_{x_{k-1}}^{x_k} f''(x)\varphi_k(x)dx = \int_a^b f''(x)\varphi(x)dx. \tag{10}$$

**Proof.** We introduce the following notations

$$I(f) := \int_a^b f(x)dx, \tag{11}$$

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

Using the property of additivity of definite integrals and taking into account equation (7), from equation (11) we obtain the following

$$\begin{gathered} I(f) = \int_a^b f(x)dx = \sum_{k=1}^{n} \int_{x_{k-1}}^{x_k} f(x)dx = \sum_{k=1}^{n} \int_{x_{k-1}}^{x_k} \varphi_k''(x) f(x)dx = \\ = \sum_{k=1}^{n} \left[ \varphi_k'(x) f(x) \Big|_{x_{k-1}}^{x_k} - \int_{x_{k-1}}^{x_k} \varphi_k'(x) f'(x)dx \right] = \\ = \sum_{k=1}^{n} \left[ \varphi_k'(x_k) f(x_k) - \varphi_k'(x_{k-1}) f(x_{k-1}) - \varphi_k(x_k) f'(x_k) + \int_{x_{k-1}}^{x_k} f''(x)\varphi_k(x)dx \right] = \\ = \sum_{k=1}^{n} \varphi_k'(x_k) f(x_k) - \sum_{k=1}^{n} \varphi_k'(x_{k-1}) f(x_{k-1}) - \sum_{k=1}^{n} \varphi_k(x_k) f'(x_k) + \\ + \sum_{k=1}^{n} \varphi_k(x_{k-1}) f'(x_{k-1}) + \sum_{k=1}^{n} \int_{x_{k-1}}^{x_k} f''(x)\varphi_k(x)dx = \\ = \sum_{k=1}^{n} \varphi_k'(x_k) f(x_k) - \sum_{k=0}^{n-1} \varphi_{k+1}(x_k) f(x_k) - \sum_{k=1}^{n} \varphi_k(x_k) f'(x_k) + \\ + \sum_{k=0}^{n-1} \varphi_{k+1}(x_k) f'(x_k) + \sum_{k=1}^{n} \int_{x_{k-1}}^{x_k} f''(x)\varphi_k(x)dx = \\ = \varphi_n'(x_n) f(x_n) + \sum_{k=1}^{n-1} \varphi_k'(x_k) f(x_k) - \varphi_1'(x_0) f(x_0) - \sum_{k=1}^{n-1} \varphi_{k+1}(x_k) f(x_k) - \end{gathered}$$

$$-\varphi_n(x_n)f'(x_n)-\sum_{k=1}^{n-1}\varphi_k(x_k)f'(x_k)+\varphi_1(x_0)f'(x_0)+\sum_{k=1}^{n-1}\varphi_{k+1}(x_k)f'(x_k)+ \\ +\sum_{k=1}^{n}\int_{x_{k-1}}^{x_k} f''(x)\varphi_k(x)dx. \tag{13}$$

From this, we obtain

$$I(f)=-\varphi_1'(x_0)f(x_0)+\sum_{k=1}^{n-1}\left(\varphi_k'(x_k)-\varphi_{k+1}'(x_k)\right)f(x_k)+\varphi_n'(x_n)f(x_n)+ \\ +\varphi_1(x_0)f'(x_0)-\sum_{k=1}^{n-1}\left(\varphi_k(x_k)-\varphi_{k+1}(x_k)\right)f'(x_k)-\varphi_n(x_n)f'(x_n)+R_n(f)= \\ =\sum_{k=0}^{n}A_{0k}f(x_k)+\sum_{k=0}^{n}A_{1k}f'(x_k)+R_n(f). \tag{14}$$

From (14), we obtain the following

$$\begin{gathered} A_{00}=-\varphi_1'(x_0), \\ A_{0k}=\varphi_k'(x_k)-\varphi_{k+1}'(x_k), \quad k=1,2,\dots,n-1, \\ A_{0n}=\varphi_n'(x_n), \\ A_{10}=\varphi_1(x_0), \\ A_{1k}=\varphi_{k+1}(x_k)-\varphi_k(x_k), \quad k=1,2,\dots,n-1, \\ A_{1n}=-\varphi_n(x_n). \end{gathered} \tag{15}$$

The error for the formula is given as follows

$$R_n(f)=\sum_{k=1}^{n}\int_{x_{k-1}}^{x_k} f''(x)\varphi_k(x)dx=\int_a^b f''(x)\varphi(x)dx. \tag{16}$$

Lemma is proved.

By determining the function $\varphi$ using equalities (15), we can compute the coefficients $A_{0k}$ and $A_{1k}$ for $k=0,\dots,n$. This approach to constructing quadrature formulas is called the $\varphi$-function method.

From equation (16), it is evident that the quadrature formula (1) is exact for any linear functions.

## 4 Optimality problem

In this section, we consider the optimality problem of the quadrature formula of the form (1) in $L_2^{(2)}(a,b)$ space. Using the Cauchy-Schwarz inequality for the absolute value of the error (16) of the quadrature formula (1), we obtain the following upper bound

$$|R_n(f)|\leqslant\sqrt{\int_a^b (f''(x))^2dx}\cdot\sqrt{\int_a^b \varphi^2(x)dx}=\|f(x)\|_{L_2^{(2)}}\cdot\|\varphi(x)\|_{L_2}. \tag{17}$$

In order to get the smallest value of $|R_n(f)|$ in the space $L_2^{(2)}$ with respect to $A_0$ and $A_1$ we should find the minimum value of the right hand side of (17) with respect to $C_k$ and $D_k$. That is to find the coefficients $A_0$ and $A_1$ of the optimal quadrature formula of the form (1) we find $C_k$ and $D_k$ that give the minimum to the norm $\|\varphi\|_{L_2}$. For this we have the following results.

**Lemma 4.1.** *For the optimal quadrature formula of the form (1) in the sense of Sard in the space $L_2^{(2)}(a,b)$, the general form of the function $\varphi_k(x)$ is given as*

$$\varphi_k(x) = \frac{x^2}{2} - \frac{x_k + x_{k-1}}{2} \cdot x + \frac{(x_k + x_{k+1})^2 + 2x_k x_{k-1}}{12}. \tag{18}$$

**Proof.** We consider the function $\varphi_k(x)$ in the interval $x \in [x_{k-1}, x_k]$, which is the solution of the following equation

$$y'' = 1. \tag{19}$$

Solving this equation gives:

$$y = \frac{x^2}{2} + Cx + D. \tag{20}$$

Thus, the function $\varphi_k(x)$ can be expressed as

$$\varphi_k(x) = \frac{x^2}{2} + C_k x + D_k. \tag{21}$$

For each $x \in [x_{k-1}, x_k]$, $\quad k = 1, 2, \ldots, n \quad$ the function $\varphi_k(x)$ is given as follows

$$\varphi_k(x) = \frac{x^2}{2} + C_k x + D_k, \quad x \in [x_{k-1}, x_k], \quad k = 1, 2, \ldots, n. \tag{22}$$

To find $\varphi_k(x)$ we need to determine the unknowns $C_k$ and $D_k$ for $k = 1, 2, \ldots, n$ that give the minimum to the right side of inequality (17). That is we consider the following quadratic function with respect to $C_k$ and $D_k$

$$F_k(C_k, D_k) = \int\limits_{x_{k-1}}^{x_k} (\varphi_k(x))^2 \, dx = \int\limits_{x_{k-1}}^{x_k} \left( \frac{x^2}{2} + C_k x + D_k \right)^2 dx, \quad k = 1, 2, \ldots, n.$$

To find the minimum of this function we take the partial derivatives of $F_k(C_k, D_k)$ with respect to $C_k$ and $D_k$ and set them to zero

$$2 \int\limits_{x_{k-1}}^{x_k} \left( \frac{x^2}{2} + C_k x + D_k \right) x dx = 0,$$

$$2 \int\limits_{x_{k-1}}^{x_k} \left( \frac{x^2}{2} + C_k x + D_k \right) dx = 0.$$

From above, we obtain the following system of two equations with two unknowns

$$\begin{cases} 2C_k \int\limits_{x_{k-1}}^{x_k} x^2 dx + 2D_k \int\limits_{x_{k-1}}^{x_k} x dx = -\int\limits_{x_{k-1}}^{x_k} x^3 dx, \\ 2C_k \int\limits_{x_{k-1}}^{x_k} x dx + 2D_k \int\limits_{x_{k-1}}^{x_k} dx = -\int\limits_{x_{k-1}}^{x_k} x^2 dx. \end{cases} \tag{23}$$

Solving this system of equations, we find the unknowns to be

$$C_k = -\frac{x_k + x_{k-1}}{2}, \tag{24}$$

$$D_k = \frac{(x_k + x_{k+1})^2 + 2x_k x_{k-1}}{12}. \tag{25}$$

Now, using (24) and (25), we can express $\varphi_k$ as

$$\varphi_k(x) = \frac{x^2}{2} - \frac{x_k + x_{k-1}}{2} \cdot x + \frac{(x_k + x_{k+1})^2 + 2x_k x_{k-1}}{12}. \tag{26}$$

Lemma is proved.

Now using (26), we have possiblity to find the coefficients $A_{0k}$ and $A_{1k}$ for $k = 0, \ldots, n$ of the optimal quadrature formula of the form (1).

The following holds.

**Theorem 4.1.** *In the space $L_2^{(2)}(a, b)$, for each fixed positive integer $n$, there is a quadrature formula that is optimal in the sense of Sard of the form*

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

with coefficients

$$A_{00} = \frac{x_1 - x_0}{2},$$

$$A_{0k} = \frac{x_{k+1} - x_{k-1}}{2}, \quad k = 1, 2, \ldots, n-1,$$

$$A_{0n} = \frac{x_n - x_{n-1}}{2},$$

$$A_{10} = \frac{(x_1 - x_0)^2}{12},$$

$$A_{1k} = \frac{1}{12}(x_{k+1} - x_{k-1})(x_{k-1} - 2x_k + x_{k+1}), \quad k = 1, 2, \ldots, n-1,$$

$$A_{1n} = \frac{(x_n - x_{n-1})^2}{12},$$

for fixed nodes $x_k$, $k = 0, 1, \ldots, n$ satisfying the inequality $a = x_0 < x_1 < \cdots < x_n = b$.

Specifically, if the nodes are equally spaced in the interval $[a, b]$ the well-known Euler-Maclaurin formula emerges.

## 5 Conclusion

In this study, we developed an optimal quadrature formula in the Sobolev space that includes derivatives and is designed for arbitrarily fixed nodes. Unlike previous approaches, where function and derivative coefficients were optimized sequentially, our method simultaneously optimizes both, ensuring greater accuracy and efficiency in numerical integration. By employing the $\varphi$ -function method, we systematically determined the quadrature coefficients that minimize the error functional in the Sard sense. This approach allowed us to construct a quadrature formula that effectively captures the underlying function behavior while incorporating derivative information, leading to improved precision in numerical integration. Furthermore, we derived explicit expressions for the quadrature coefficients and analyzed their properties. Our results demonstrate that when the nodes are evenly distributed in the interval $[a, b]$, the derived formula coincides with the well-known Euler-Maclaurin formula, reinforcing the validity of our approach. Overall, this work contributes to the theory of quadrature formulas by introducing a refined method for constructing optimal formulas in Sobolev spaces. Future research may focus on extending this approach to higher-order derivatives and exploring its applications in solving practical problems in applied mathematics, physics, and engineering.

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# ОПТИМАЛЬНАЯ КВАДРАТУРНАЯ ФОРМУЛА С ПРОИЗВОДНЫМИ ДЛЯ ПРОИЗВОЛЬНО ФИКСИРОВАННЫХ УЗЛОВ В ПРОСТРАНСТВЕ СОБОЛЕВА

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Численное вычисление определенных интегралов играет важную роль в различных прикладных и теоретических дисциплинах. Во многих случаях точная аналитическая оценка интегралов невозможна из-за сложности подынтегральной функции или характера пределов интегрирования. Квадратурные формулы обеспечивают эффективный подход к аппроксимации определенных интегралов, основываясь на взвешенных суммах значений функции в выбранных узлах. Традиционные квадратурные формулы, такие как формулы Ньютона-Котса, Гаусса, направлены на повышение точности путем тщательного выбора узлов и весов. Однако оптимальные квадратурные формулы также могут быть построены в смысле Сарда, минимизируя норму функционала ошибки в заданном функциональном пространстве. В данной работе мы сосредотачиваемся на построении оптимальной квадратурной формулы в пространстве Соболева с произвольно фиксированными узлами. В отличие от традиционных подходов, где коэффициенты определяются последовательно, мы одновременно оптимизируем как коэффициенты функции, так и коэффициенты её производной, что улучшает общую точность и стабильность. Вывод формулы основан на методе $\varphi$-функций, который позволяет явно выражать коэффициенты квадратурной формулы и анализировать их свойства ошибки. Полученная квадратурная формула минимизирует норму ошибки в выбранном функциональном пространстве, обеспечивая улучшенную аппроксимацию определенных интегралов. Кроме того, если узлы равномерно распределены, наши результаты приводят к хорошо известной формуле Эйлера-Маклорена, что демонстрирует эффективность нашего подхода.

**Ключевые слова:** квадратурная формула, пространство Соболева, оптимальная аппроксимация, метод $\varphi$-функций, формула Эйлера-Маклорена.

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