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OPTIMAL QUADRATURE FORMULA IN THE SPACE OF DIFFERENTIABLE FUNCTIONS

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English VersionNumerical integration in Sobolev spaces often relies on optimal quadrature formulas in the sense of Sard to minimize the calculation error. While many standard formulas exist, constructing optimal rules that incorporate a specific combination of data—such as function values at nodes, first-order derivatives at interval boundaries, and third-order derivatives at nodes—presents a complex mathematical challenge, as previous studies lack an explicit framework for deriving exact analytical coefficients. The primary objective of this study is to construct optimal quadrature formulas in the sense of Sard by minimizing the error functional with these mixed derivative data. The study employs a variational method to construct the formula: an analytical expression for the norm of the error functional is first derived, the Lagrange multiplier method is applied to generate a Wiener–Hopf type system of linear equations, and the Sobolev method is utilized to extract the exact analytical form of the optimal coefficients. Through the applied approach, precise analytical expressions for optimal quadrature coefficients are successfully obtained, and the coefficients for the spaces $L_2^{(4)}(0,1)$ and $L_2^{(5)}(0,1)$ are fully calculated as an exact application. The explicit solution confirms that the newly found coefficients strictly minimize the error functional, significantly enhancing the mathematical toolkit for numerical integration in Sobolev spaces.

Keywords: Sobolev space, optimal quadrature formula, error function, extremal function, optimal coefficients

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1 Introduction

Many practical problems in applied sciences and mathematical physics are expressed in the form of integrals. Numerical integration methods are sometimes referred to as quadrature rules, as they are used to approximate the integrals of single-variable functions. Because quadrature rules enable the high-precision estimation of an integral's true value even in the most complex problems, the numerical evaluation of integrals using these methods continues to be a primary direction of mathematical research. These formulas are used to calculate the area of a region defined by a function that is integrable over a finite or infinite interval. If the integrable function cannot be integrated analytically, or if it lacks a precise mathematical expression and its values are only given in tabular form, then numerical integration is the only solution [1–4].

In some cases, classical quadrature formulas do not fully account for the properties of the function under the integral. Therefore, the issues of further improvement of quadrature formulas, increasing their accuracy and minimizing errors are becoming relevant. Derivative quadrature formulas involve not only the values of a function but also its first-order or higher-order derivatives. Formulas of this type yield effective results in the numerical solution of differential equations, variational calculus, and the approximate integration of smooth functions.

The effectiveness of quadrature rules is typically determined by the degree of accuracy and the order of convergence. Therefore, achieving a high degree of accuracy and order of convergence in numerical integration formulas is one of the primary tasks in the field of numerical analysis.

There are numerous methods for constructing optimal quadrature and cubature formulas for the approximate calculation of definite integrals of functions defined in Banach spaces. These include the Sobolev method [1, 2], the spline-function method, and the φ-function method. In recent years, a number of new approaches have been proposed in this field to enhance computational efficiency and adapt to special classes of functions. In particular, K.P. Lovetskiy et al. [5] proposed a specific approach based on the Levin algorithm for computing integrals of highly oscillatory functions. J.A. Rivera and co-authors [6] analyzed various quadrature problems, including Monte Carlo methods, through 1D numerical examples while solving partial differential equations using neural networks. Furthermore, M. Gnewuch et al. [7] demonstrated that quasi-Monte Carlo (QMC) integration based on arbitrary (t, m, s)-nets yields optimal convergence rates in various function spaces. Quadrature rules are also widely used in the approximate solution of integral equations. For instance, S. Micula [8] conducted a thorough analysis of iterative methods for Fredholm–Hammerstein integral equations with modified arguments. Aiming to improve the computational efficiency—in terms of both time and cost—of traditional methods, S. Mahesar et al. [9] developed new and efficient quadrature rules based on the combinations of the function and its first derivative evaluations at equally spaced data points. Building upon the recent studies mentioned above and the traditional approaches of scholars such as S.L. Sobolev, S.M. Nikolskiy, N.P. Korneichuk, and A.A. Zhensykbaev, scientists in our republic have also achieved significant results. Specifically, Kh.M. Shadimetov [10, 11], A.R. Hayotov [12], F.A. Nuraliev [13–16], and others [17–19] have conducted extensive research on constructing optimal quadrature and cubature formulas for the error functional in various spaces, such as $L_2^{(m)}$.

The remainder of the article is organized as follows. Section 2 describes the problem of constructing a quadrature formula. In Section 3, a general expression for the norm of the error functional is derived using an extremal function. In Section 4, a system of linear equations of the Wiener–Hopf type is obtained for the coefficients of the quadrature formula under consideration in the $L_2^{(m)}(0, 1)$ space. In Section 5, analytical expressions for the optimal coefficients of the quadrature formula with derivatives are found for the cases of $m = 4$ and $m = 5$.

2 Problem statement

In this work, we consider the problem of constructing a quadrature formula as follows

$$\int_0^1 f(x)dx \cong \sum_{\beta=0}^{N} K_0[\beta] f(h\beta) + \frac{h^2}{12}(f'(0) - f'(1)) + \sum_{\beta=0}^{N} K_1[\beta] f'''(h\beta), \tag{1}$$

where $K_0[\beta] = \begin{cases} h/2\,; & \beta = 0, N, \\ h; & \beta = \overline{1, N-1}, \end{cases}$ $K_1[\beta]$ are unknown coefficients of the quadrature formula (1), $f \in L_2^{(m)}(0,1)$, N is a natural number, $h = \frac{1}{N}$, $L_2^{(m)}(0,1)$ is the space of quadratically integrable functions with a generalized derivative of order m.

The difference between the exact value of the integral and the approximate value obtained from the quadrature formula is called the error of the quadrature formula and its is determined as follows

$$\begin{gathered} \int_0^1 f(x)dx - \sum_{\beta=0}^{N} K_0[\beta]f(h\beta) - \frac{h^2}{12}(f'(0) - f'(1)) - \sum_{\beta=0}^{N} K_1[\beta]f'''(h\beta) = \\ = \int_0^1 l_N(x)f(x)dx = (l_N, f)\,. \end{gathered} \tag{2}$$

The following error functional corresponds to the difference (2)

$$\begin{gathered} l_N(x) = \varepsilon_{[0,1]}(x) - \sum_{\beta=0}^{N} K_0[\beta]\delta\left(x - h\beta\right) + \frac{h^2}{12}\left(\delta'(x) - \delta'(x-1)\right) + \\ + \sum_{\beta=0}^{N} K_1[\beta]\delta'''\left(x - h\beta\right), \end{gathered} \tag{3}$$

where $\delta(x)$ is Dirac's delta-function, $\varepsilon_{[0,1]}(x)$ is the characteristic function of the interval [0,1].

The norm in the space $L_2^{(m)}(0,1)$ is defined as follows

$$\|u\|^2_{L_2^{(m)}(0,1)} = \int_0^1 \left(u^{(m)}(x)\right)^2 dx.$$

Furthermore, the error functional (3) is required to satisfy the following conditions

$$(l_N, x^\alpha) = 0, \;\; \alpha = \overline{0, m-1}. \tag{4}$$

Based on the Cauchy–Schwarz inequality, the error (2) is estimated as follows

$$|(l_N, f)| \leqslant ||f||_{L_2^{(m)}} \cdot \|l_N\|_{L_2^{(m)*}}. \tag{5}$$

The error functional depends on the coefficients $K_1[\beta]$, $\beta = 0, 1, ..., N$ and the node points $h\beta$. We find the minimum of the norm of the error functional (3) with respect to the coefficients $K_1[\beta]$ while the node points are fixed, that is we find the following quantity

$$\left\|\bar{l}_N\right\|_{L_2^{*(m)}} = \inf_{K_1[\beta]} \|l_N\|_{L_2^{*(m)}}. \tag{6}$$

The coefficients satisfying equality (6) are called optimal coefficients, and the corresponding quadrature formula is called the optimal quadrature formula.

First, let us consider the following problem.

Problem A. To determine the general form of the norm of the error functional $l_N(x)$ of type (3).

In the following section, our main task is to determine the norm of the error functional, that is, to solve problem A.

3 The norm of the error functional

To determine the general form of the norm of the error functional, we use the Riesz representation theorem concerning the general form of a linear, continuous functional in a Hilbert space [1,4]. For any linear, continuous functional $l_N(x)$ defined in the space $L_2^{(m)}(0,1)$, there exists an element $\psi_{l_N}(x) \in L_2^{(m)}(0,1)$ such that the following equalities hold for all $f \in L_2^{(m)}(0,1)$

$$(l_N, f) = \langle \psi_{l_N}, f \rangle ,$$
$$\|l_N\|_{L_2^{(m)*}} = \|\psi_{l_N}\|_{L_2^{(m)}},$$

where

$$\langle \psi_{l_N}, f \rangle = \int_0^1 \psi_{l_N}^{(m)}(x) f^{(m)}(x)dx.$$

According to Riesz's theory, to determine the general form of the norm for the error functional (3), we need to define the function $\psi_{l_N}(x)$. To achieve this, we will use the concept of an extremal function, introduced by S.L. Sobolev [1]. In the space $L_2^{(m)}(0,1)$, the extremal function $\psi_{l_N}(x)$ corresponding to the error functional $l_N(x)$ has the following form

$$\psi_{l_N}(x) = (-1)^m l_N(x) * \frac{x^{2m-1}\operatorname{sign} x}{2(2m-1)!} + P_{m-1}(x), \tag{7}$$

where $P_{m-1}(x)$ is an algebraic polynomial of degree $(m-1)$.

The following equality holds for the norm of the error functional in the space $L_2^{(m)}(0,1)$

$$\|l_N\|^2_{L_2^{(m)*}} = (l_N, \psi_{l_N}) = \left(l_N(x), \left((-1)^m l_N(x) * \frac{x^{2m-1}\operatorname{sign} x}{2(2m-1)!} + P_{m-1}(x) \right) \right). \tag{8}$$

After some calculations, for the square of the norm of the error functional (8), we have the following

$$\begin{gathered}
\|l_N\|^2 = (-1)^m \left\{ -\sum_{\beta=0}^{N}\sum_{\gamma=0}^{N} K_1[\beta]K_1[\gamma]\frac{(h\gamma-h\beta)^{2m-7}}{2(2m-7)!}\operatorname{sign}(h\gamma-h\beta) - \right. \\
+2\sum_{\beta=0}^{N} K_1[\beta]\sum_{\gamma=0}^{N} K_0[\gamma]\frac{(h\beta-h\gamma)^{2m-4}}{2(2m-4)!}\operatorname{sign}(h\beta-h\gamma) + \\
+2\sum_{\beta=0}^{N} K_1[\beta]\int_0^1 \frac{(x-h\beta)^{2m-4}}{2(2m-4)!}\operatorname{sign}(x-h\beta)dx - 2\cdot\frac{h^2}{12}\sum_{\beta=0}^{N} K_1[\beta]\left(\frac{(h\beta)^{2m-5}}{2(2m-5)!} - \right. \\
\left. -\frac{(1-h\beta)^{2m-5}}{2(2m-5)!} \right) - \frac{h^2}{6}\sum_{\beta=0}^{N} K_0[\beta]\left(\frac{(h\beta)^{2m-2}}{2(2m-2)!} + \frac{(1-h\beta)^{2m-2}}{2(2m-2)!} \right) + \\
+\sum_{\gamma=0}^{N}\sum_{\beta=0}^{N} K_0[\gamma]K_0[\beta]\frac{(h\gamma-h\beta)^{2m-1}}{2(2m-1)!}\operatorname{sign}(h\gamma-h\beta) - \\
\left. -2\sum_{\beta=0}^{N} K_0[\beta]\int_0^1 \frac{(x-h\beta)^{2m-1}}{2(2m-1)!}\operatorname{sign}(x-h\beta)dx + \frac{h^2}{6(2m-1)!} + \frac{1}{(2m+1)!} \right\}.
\end{gathered} \tag{9}$$

Consequently, problem A is completely solved.

Now we come to the following problem.

Problem B. Finding the coefficients $K_1[\beta],\ \beta=0,1,2,...,N$ that yield the minimum value of the quadratic function (9).

Now we will deal with finding the unknown coefficients $K_1[\beta],\ \beta=0,1,2,...,N$.

4 The system for optimal coefficients

In this section, a system is derived that allows for the determination of optimal coefficients.

From equality (9), the square of the norm of the error functional $\|l_N\|^2_{L_2^{(m)*}}$ is a quadratic function of $N+1$ variables with respect to the coefficients $K_1[\beta]$, $\beta = 0,1,,...,N$. To find the extremum of this function, we use the Lagrange method of undetermined multipliers. Taking condition (4) into account, we construct the following Lagrange function

$$\Lambda\left(K_1[0],K_1[1],...,K_1[N],\lambda_3,...,\lambda_{m-1}\right)=\|l_N\|^2+2(-1)^m\sum_{\alpha=3}^{m-1}\lambda_\alpha(l_N,x^\alpha), \tag{10}$$

where λ_α, $\alpha=\overline{3,m-1}$ represents the unknown multipliers. Here, the cases $\alpha=0,1,2$ are satisfied by the values of the function and the coefficients in the first-order derivative. By setting the partial derivatives of the function (10) with respect to the λ_α, $\alpha=\overline{3,m-1}$ unknown multipliers and the $K_1[\beta]$, $\beta=\overline{0,N}$ coefficients to zero, we obtain the following system of linear algebraic equations

$$\begin{gathered}\sum_{\gamma=0}^{N}K_1[\gamma]\frac{(h\beta-h\gamma)^{2m-7}}{2(2m-7)!}\operatorname{sign}(h\beta-h\gamma)+P_{m-4}(h\beta)=\\=\sum_{j=0}^{2m-7}\frac{(h\beta)^{2m-7-j}}{(2m-7-j)!}\left[\frac{B_{j+4}h^{j+4}}{(j+4)!}+\sum_{i=1}^{j}\frac{(-1)^jB_{j+4-i}h^{j+4-i}}{2i!(j+4-i)!}\right],\quad \beta=\overline{0,N}\end{gathered} \tag{11}$$

$$\sum_{\beta=0}^{N}K_1[\beta](h\beta)^\alpha=-\sum_{i=1}^{\alpha}\frac{\alpha!B_{\alpha+4-i}h^{\alpha+4-i}}{i!(\alpha+4-i)!};\quad \alpha=\overline{0,m-4}\,, \tag{12}$$

where $P_{m-4}(h\beta)$ is an unknown polynomial of degree $m-4$, $B_i,\ \ i=1,2,...$ are Bernoulli numbers.

In the solution $\overset{\circ}{K}{}_1[\beta],\ \beta=\overline{0,N},\ \overline{\lambda}_\alpha,\ \alpha=\overline{3,m-1}$ of the system (11)–(12), the function (9) reaches its minimum value at this point because the quadratic form, composed of the second-order partial derivatives of the Lagrange function with respect to all variables, is positive definite. Therefore, by finding the solution to the system (11)–(12), we will have determined the optimal coefficients that give the minimum value to the norm of the error functional (3). In the system of equations (11)–(12), the coefficients $K_1[\beta],\ \beta=\overline{0,N}$ and the polynomial $P_{m-4}(h\beta)$ are unknowns. This system of equations will have a unique solution that yields the minimum value for the norm $\|l_N\|^2_{L_2^{(m)*}}$.

5 Calculating coefficients of optimal quadrature formula

Now we solve the system of equations (11)–(12) in the space $L_2^{(m)}(0,1)$ for cases $m=4$ and $m=5$ and have the following theorem.

Theorem 1. *The coefficients of the quadrature formula with derivatives of the form* (1) *in the spaces* $L_2^{(4)}(0,1), L_2^{(5)}(0,1)$ *are as follows*

$$\begin{aligned} K_1[0] &= -\frac{h^4}{720}, \\ K_1[\beta] &= 0, \quad \beta = \overline{1, N-1}, \\ K_1[N] &= \frac{h^4}{720}. \end{aligned} \tag{13}$$

Proof. Let us consider the proof of this theorem for the space $L_2^{(5)}(0,1)$. Let us rewrite the system (11)–(12) for $m=5$

$$\begin{gathered} \sum_{\gamma=0}^{N} K_1[\gamma] \frac{(h\beta - h\gamma)^3}{12} \operatorname{sign}(h\beta - h\gamma) + P_1(h\beta) = \\ = \frac{h^4}{1440}\left(\frac{1}{6} - \frac{(h\beta)}{2} + \frac{(h\beta)^2}{2} - \frac{(h\beta)^3}{3}\right) + \frac{h^6}{30240}\left(h\beta - \frac{1}{2}\right), \quad \beta = \overline{0, N}. \end{gathered} \tag{14}$$

$$\sum_{\beta=0}^{N} K_1[\beta] = 0, \tag{15}$$

$$\sum_{\beta=0}^{N} K_1[\beta](h\beta) = \frac{h^4}{720}, \tag{16}$$

where $P_1(h\beta)$ is an unknown polynomial of degree 1.

To solve the system (14)–(16), we use the discrete analog of the differential operator $\frac{d^4}{dx^4}$ (see [10])

$$D_2(h\beta) = \frac{6}{h^4} \begin{cases} 6\sqrt{3} q^{|\beta|}, & |\beta| \geqslant 2, \\ 19 - 12\sqrt{3}, & |\beta| = 1, \\ 6\sqrt{3} - 8, & \beta = 0. \end{cases} \tag{17}$$

Here $q = \sqrt{3} - 2$. For the values $\beta < 0$ and $\beta > N$, $K_1[\beta] = 0$.

Let us rewrite equation (14) in a convoluted form

$$\begin{gathered} K_1[\beta] * \frac{(h\beta)^3}{6} \operatorname{sign}(h\beta) + P_1(h\beta) = \\ = \frac{h^4}{1440}\left(\frac{1}{6} - \frac{(h\beta)}{2} + \frac{(h\beta)^2}{2} - \frac{(h\beta)^3}{3}\right) + \frac{h^6}{30240}\left(h\beta - \frac{1}{2}\right), \ \beta = \overline{0, N}. \end{gathered} \tag{18}$$

Let us denote the left and right sides of equation (18) as follows

$$u(h\beta) = K_1[\beta] * \frac{(h\beta)^3}{6} \operatorname{sign}(h\beta) + P_1(h\beta),$$

$$w(h\beta) = \frac{h^4}{1440}\left(\frac{1}{6} - \frac{(h\beta)}{2} + \frac{(h\beta)^2}{2} - \frac{(h\beta)^3}{3}\right) + \frac{h^6}{30240}\left(h\beta - \frac{1}{2}\right), \ \beta = \overline{0, N}.$$

Considering the properties of the differential operator $D_2(h\beta)$ (see [10]), we obtain the following

$$K_1[\beta] = D_2(h\beta) * u(h\beta) = D_2(h\beta) * \left(K_1[\beta] * \frac{(h\beta)^3}{6} \operatorname{sign}(h\beta) + P_1(h\beta) \right) =$$

$$= K_1[\beta] * \left(D_2(h\beta) * \frac{(h\beta)^3}{6} \operatorname{sign}(h\beta) \right) = K_1[\beta] * \delta(h\beta) = K_1[\beta].$$

Now, let's determine the values of the function $u(h\beta)$ for all integer values of β. When $\beta = \overline{0, N}$, $u(h\beta) = w(h\beta)$. When $\beta < 0$ we have

$$u(h\beta) = -\frac{(h\beta)^3}{12} \sum_{\gamma=0}^{N} K_1[\gamma] + \frac{(h\beta)^2}{4} \sum_{\gamma=0}^{N} K_1[\gamma](h\gamma) -$$

$$-\frac{(h\beta)}{4} \sum_{\gamma=0}^{N} K_1[\gamma](h\gamma)^2 + \frac{1}{12} \sum_{\gamma=0}^{N} K_1[\gamma](h\gamma)^3 + P_1(h\beta) = Q_1^-(h\beta).$$

At $\beta > N$

$$u(h\beta) = \frac{(h\beta)^3}{12} \sum_{\gamma=0}^{N} K_1[\gamma] - \frac{(h\beta)^2}{4} \sum_{\gamma=0}^{N} K_1[\gamma](h\gamma) +$$

$$+\frac{(h\beta)}{4} \sum_{\gamma=0}^{N} K_1[\gamma](h\gamma)^2 - \frac{1}{12} \sum_{\gamma=0}^{N} K_1[\gamma](h\gamma)^3 + P_1(h\beta) = Q_1^+(h\beta).$$

Thus, the function $u(h\beta)$ has the following form

$$u(h\beta) = \begin{cases} Q_1^-(h\beta), & \beta < 0, \\ w(h\beta), & \beta = \overline{0, N}, \\ Q_1^+(h\beta), & \beta > N, \end{cases} \tag{19}$$

where $Q_1^-(h\beta)$, $Q_1^+(h\beta)$ are unknown polynomials of degree 1.

First, we will find the values of $K_1[\beta]$, $\beta = 1, 2, ..., N-1$

$$K_1[\beta] = D_2(h\beta) * u(h\beta) = \sum_{\gamma=-\infty}^{\infty} D_2(h\beta - h\gamma) u(h\gamma) =$$

$$= \sum_{\gamma=-\infty}^{-1} D_2(h\beta - h\gamma) u(h\gamma) + \sum_{\gamma=0}^{N} D_2(h\beta - h\gamma) u(h\gamma) + \sum_{\gamma=N+1}^{\infty} D_2(h\beta - h\gamma) u(h\gamma) =$$

$$= \sum_{\gamma=1}^{\infty} D_2(h\beta + h\gamma) u(-h\gamma) + D_2(h\beta) w(h\beta) + \sum_{\gamma=1}^{\infty} D_2(h\beta - h(\gamma + N)) u(h(\gamma + N)).$$

From the last equality, taking into account the form (17) of the differential operator $D_2(h\beta)$ and equality (19), we have

$$K_1[\beta] = h^4 q^\beta \sum_{\gamma=1}^{\infty} \frac{36\sqrt{3} q^\gamma}{h^8} \left(Q_1^-(-h\gamma) - w(-h\gamma) \right) +$$

$$+h^4 q^{N-\beta} \sum_{\gamma=1}^{\infty} \frac{36\sqrt{3}q^{\gamma}}{h^8} \left(Q_1^+(h(\gamma+N)) - w(h(\gamma+N)) \right).$$

From this, we obtain the following result

$$K_1[\beta] = h^4 \left(aq^{\beta} + bq^{N-\beta} \right), \quad \beta = \overline{1, N-1}, \tag{20}$$

where

$$a = \sum_{\gamma=1}^{\infty} \frac{36\sqrt{3}q^{\gamma}}{h^8} \left(Q_1^-(-h\gamma) - w(-h\gamma) \right),$$

$$b = \sum_{\gamma=1}^{\infty} \frac{36\sqrt{3}q^{\gamma}}{h^8} \left(Q_1^+(h(\gamma+N)) - w(h(\gamma+N)) \right).$$

Now, we will find a and b. To do this, we can write the sum in equation (14) as follows

$$S(h\beta) = \sum_{\gamma=0}^{N} K_1[\gamma] \frac{(h\beta - h\gamma)^3}{12} = K_1[0] \frac{(h\beta)^3}{6} + S_1(h\beta) - S_2(h\beta), \tag{21}$$

$$S_1(h\beta) = \sum_{\gamma=1}^{\beta-1} K_1[\gamma] \frac{(h\beta - h\gamma)^3}{6} = \sum_{\gamma=1}^{\beta-1} h^4 \left(aq^{\gamma} + bq^{N-\gamma} \right) \frac{(h\beta - h\gamma)^3}{6} =$$

$$= \frac{h^7}{6} \sum_{\gamma=1}^{\beta-1} \left(aq^{\beta-\gamma} + bq^{N-\beta+\gamma} \right) \gamma^3 = \frac{h^7}{6} \left(aq^{\beta} \sum_{\gamma=1}^{\beta-1} q^{-\gamma}\gamma^3 + bq^{N-\beta} \sum_{\gamma=1}^{\beta-1} q^{\gamma}\gamma^3 \right).$$

To calculate the value of $S_1(h\beta)$, we use the following formula [20]

$$\sum_{\gamma=0}^{n-1} q^{\gamma}\gamma^k = \frac{1}{1-q} \sum_{i=0}^{k} \left(\frac{q}{1-q} \right)^i \Delta^i 0^k - \frac{q^n}{1-q} \sum_{i=0}^{k} \left(\frac{q}{1-q} \right)^i \Delta^i n^k.$$

After some calculations, we get the following result

$$S_1(h\beta) = -\sum_{j=0}^{3} \frac{(h\beta)^{3-j} h^{j+4}}{j!(3-j)!} \sum_{i=0}^{j} \frac{aq + bq^{N+i}(-1)^{i+1}}{(q-1)^{i+1}} \Delta^i 0^j. \tag{22}$$

Now let's calculate $S_2(h\beta)$.

$$\begin{aligned} S_2(h\beta) &= \sum_{\gamma=0}^{N} K_1[\gamma] \frac{(h\beta - h\gamma)^3}{12} = \sum_{\gamma=0}^{N} K_1[\gamma] \sum_{j=0}^{3} \frac{(h\beta)^{3-j}(h\gamma)^j(-1)^j}{2j!(3-j)!} = \\ &= -\frac{h^4(h\beta)^2}{2880} + \frac{h\beta}{4} \sum_{\gamma=0}^{N} K_1[\gamma](h\gamma)^2 - \frac{1}{12} \sum_{\gamma=0}^{N} K_1[\gamma](h\gamma)^3. \end{aligned} \tag{23}$$

Using (21), (22), (23) in equation (14), we obtain

$$\begin{aligned} &K_1[0] \frac{(h\beta)^3}{6} - \sum_{j=0}^{3} \frac{(h\beta)^{3-j} h^{j+4}}{j!(3-j)!} \sum_{i=0}^{j} \frac{aq + bq^{N+i}(-1)^{i+1}}{(q-1)^{i+1}} \Delta^i 0^j + \frac{h^4(h\beta)^2}{2880} - \\ &- \frac{h\beta}{4} \sum_{\gamma=0}^{N} K_1[\gamma](h\gamma)^2 + \frac{1}{12} \sum_{\gamma=0}^{N} K_1[\gamma](h\gamma)^3 + P_1(h\beta) = \\ &= \frac{h^4}{1440} \left(\frac{1}{6} - \frac{(h\beta)}{2} + \frac{(h\beta)^2}{2} - \frac{(h\beta)^3}{3} \right) + \frac{h^6}{30240} \left(h\beta - \frac{1}{2} \right). \end{aligned} \tag{24}$$

In equation (24), we equate the coefficients of $(h\beta)^3$. As a result, we obtain the value $K_1[0]$

$$K_1[0] = -\frac{h^4}{720} + h^4\frac{aq - bq^N}{q-1}. \tag{25}$$

In equation (24), we equate the coefficients of $(h\beta)^2$

$$-\frac{h^5(h\beta)^2}{2}\sum_{i=0}^{1}\frac{aq + bq^{N+i}(-1)^{i+1}}{(q-1)^{i+1}}\Delta^i 0^1 + \frac{h^4(h\beta)^2}{2880} = \frac{h^4(h\beta)^2}{2880}.$$

From here

$$\sum_{i=0}^{1}\frac{aq + bq^{N+i}(-1)^{i+1}}{(q-1)^{i+1}}\Delta^i 0^1 = 0. \tag{26}$$

Taking into account (20), (25) in equality (15), we find the value of $K_1[N]$.

$$\sum_{\gamma=0}^{N} K_1[\gamma] = 0.$$

$$h^4\left(-\frac{h^4}{720} + \frac{aq - bq^N}{q-1}\right) + h^4\sum_{\gamma=1}^{N-1}\left(aq^\gamma + bq^{N-\gamma}\right) + K_1[N] = 0.$$

Here we calculate the following

$$\sum_{\gamma=1}^{N-1} q^\gamma = \frac{q^N - q}{q-1}, \sum_{\gamma=1}^{N-1} q^{N-\gamma} = \frac{q^N - q}{q-1}. \tag{27}$$

Considering (27), for $K_1[N]$ we have the following:

$$K_1[N] = \frac{h^4}{720} - h^4\frac{aq^N - bq}{q-1}. \tag{28}$$

Equality (16) is written using equality (20), (28) as follows

$$\sum_{\gamma=0}^{N} K_1[\gamma](h\gamma) = \frac{h^4}{720} - h^4\frac{aq^N - bq}{q-1} + h^4\sum_{\gamma=1}^{N-1}\left(aq^\gamma + bq^{N-\gamma}\right)(h\gamma) = \frac{h^4}{720}.$$

From here

$$\begin{aligned}&\frac{h^4}{720} - h^4\frac{aq^N - bq}{q-1} + h^5\sum_{i=0}^{1}\frac{aq^i + bq^{N+i}(-1)^{i+1}}{(1-q)^{i+1}}\Delta^i 0^1 - \\ &-\sum_{p=0}^{1}\frac{h^{p+4}}{p!(1-p)!}\sum_{i=0}^{p}\frac{aq^{N+i} + bq(-1)^{i+1}}{(1-q)^{i+1}}\Delta^i 0^p = \frac{h^4}{720}.\end{aligned} \tag{29}$$

In equality (29), we write out the cases for $p = 0$ and $p = 1$ separately.

$$\begin{aligned}&-h^4\frac{aq^N - bq}{q-1} + h^5\sum_{i=0}^{1}\frac{aq^i + bq^{N+i}(-1)^{i+1}}{(1-q)^{i+1}}\Delta^i 0^1 - h^4\frac{aq^N - bq}{1-q} - \\ &-h^5\sum_{i=0}^{1}\frac{aq^{N+i} + bq(-1)^{i+1}}{(1-q)^{i+1}}\Delta^i 0^1 = 0.\end{aligned} \tag{30}$$

From equations (26) and (30), it follows that $a = b = 0$.

From equations (20), (25), (26), we obtain the following result

$$\begin{aligned} K_1[0] &= -\frac{h^4}{720}, \\ K_1[\beta] = 0, \quad \beta &= \overline{1, N-1}, \\ K_1[N] &= \frac{h^4}{720}. \end{aligned} \tag{31}$$

For the space $L_2^{(4)}(0,1)$, the theorem is proved in the same way.

Theorem 1 is completely proven.

6 Numerical results

To validate the theoretical results obtained in the previous sections and demonstrate the computational efficiency of the proposed optimal quadrature formula (1), we perform numerical evaluations for test integrals. Specifically, we consider the following integral:

$$I_1 = \int_0^1 f_1(x)dx,$$

where the integrand function is given by

$$f_1(x) = \sin(x^2) + e^{-x}.$$

The numerical calculation of I_1 is performed in the space $L_2^{(4)}(0,1)$. The computations are carried out for various numbers of grid subdivisions, namely $N = 10, 50, 100$, and 150. To illustrate the accuracy of our approach, the absolute errors obtained by the proposed optimal quadrature formula (denoted as OQF3) are compared with the results of existing optimal formulas from the literature [13, 14] (OQF1 and OQF2).

Table 1 Comparison of absolute integration errors for I_1 in $L_2^{(4)}(0,1)$ across different optimal quadrature formulas.

N	I_1 (exact value)	$\lvert I_1 - \text{OQF1}\rvert$	$\lvert I_1 - \text{OQF2}\rvert$	$\lvert I_1 - \text{OQF3}\rvert$
10	0.942388860552	1.331×10^{-7}	8.982×10^{-8}	2.883×10^{-9}
50	0.942388860552	3.985×10^{-11}	2.741×10^{-11}	1.857×10^{-13}
100	0.942388860552	1.234×10^{-12}	8.531×10^{-13}	3.108×10^{-15}
150	0.942388860552	1.620×10^{-13}	1.122×10^{-13}	1.110×10^{-16}

As observed from Table 1, the proposed quadrature formula OQF3 achieves significantly smaller absolute errors compared to OQF1 and OQF2 for all selected grid nodes, confirming its higher accuracy and faster convergence rate in the corresponding Sobolev space.

7 Conclusion

The quadrature formula considered in this research paper describes the integration process by approximating the values of the function at the nodes, as well as the values of its derivatives up to the third order at the nodes. In the process of determining the optimal coefficients, the problem of minimizing the value of the norm of the error functional in the Sobolev space $L_2^{(m)}(0,1)$ was posed. A system of equations was obtained that allows for the determination of optimal coefficients using the orthogonality condition, the general form of the error functional norm, and the Lagrange undetermined multipliers method. Using Sobolev's method based on the discrete analogue of the differential operator, the values of the optimal coefficients in the spaces $L_2^{(4)}(0,1)$ and $L_2^{(5)}(0,1)$ were determined, and the corresponding theorem was proven.

In conclusion, it should be noted that the quadrature formulas with derivatives of the form (1), constructed in the $L_2^{(4)}(0,1)$ and $L_2^{(5)}(0,1)$ spaces, have the same form and are optimal in these spaces.

Declarations

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Author contributions. F.A. Nuraliev: problem statement; R.M. Edilbekova: proof of the theorem and numerical experimentation.

Data availability. The data are available from the authors on reasonable request.

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ОПТИМАЛЬНАЯ КВАДРАТУРНАЯ ФОРМУЛА В ПРОСТРАНСТВЕ ДИФФЕРЕНЦИРУЕМЫХ ФУНКЦИЙ

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Численное интегрирование в пространствах Соболева часто основывается на оптимальных по Сарду квадратурных формулах, позволяющих минимизировать погрешность вычислений. Хотя существует множество стандартных формул, построение оптимальных правил, использующих комбинацию значений функции в узлах, первой производной на концах интервала и третьей производной в узлах, представляет собой сложную задачу из-за отсутствия явного аппарата для вывода аналитических коэффициентов. Основная цель данного исследования — построить такие оптимальные по Сарду формулы путем минимизации функционала погрешности. Для этого применяется вариационный подход: выводится аналитическое выражение для нормы функционала погрешности, методом множителей Лагранжа формируется система уравнений типа Винера — Хопфа, а затем методом Соболева находится точный аналитический вид оптимальных коэффициентов. С помощью предложенного метода были успешно получены формулы для коэффициентов и полностью рассчитаны их значения для пространств $L_2^{(4)}(0,1)$ и $L_2^{(5)}(0,1)$. Явное решение подтверждает, что найденные коэффициенты строго минимизируют функционал погрешности, расширяя существующий математический аппарат численного интегрирования в пространствах Соболева.

Ключевые слова: пространство Соболева, оптимальная квадратурная формула, функция погрешности, экстремальная функция, оптимальные коэффициенты

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