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OPTIMAL QUADRATURE FORMULA WITH MULTIPLE NODES IN A HILBERT SPACE

^{1,2}*Polvonov S.Z.*

szpolvonov@gmail.com

¹V.I. Romanovskiy Institute of Mathematics, Uzbekistan Academy of Sciences, 9, University str., Tashkent, 100174 Uzbekistan;²Tashkent International University, 7, Kichik khalka yoli str., Tashkent, 100084 Uzbekistan

Background: Quadrature formulas that use derivative values alongside function values attain a higher order of accuracy for a fixed number of nodes. In the variational setting of Sard the nodes are fixed in advance and only the weights are chosen, so as to minimize the norm of the error functional over a normed space of integrands. Constructions of this kind have been carried out mainly in Sobolev spaces whose seminorm is generated by a pure derivative of order m , which yields exactness on polynomials only, and the derivative weights have usually been retained at the endpoints of the interval alone.

Purpose: The aim of the work is to construct an optimal quadrature formula in the sense of Sard in the Hilbert space $W_{2,\sigma}^{(3,2)}(0,1)$ in which the first-derivative weights are retained at every node, while the function-value weights are fixed to those of the trapezoidal rule, so that exactness for the constant, the linear function and a decaying exponential is built into the formula.

Method: The construction follows the method of S.L. Sobolev. The extremal function of the error functional is determined, and the Riesz representation theorem then yields a closed-form expression for the square of the norm of that functional as a quadratic function of the unknown derivative weights. Minimizing this quadratic under the exactness constraints by the method of Lagrange multipliers leads to a linear algebraic system for the weights and the multipliers.

Results: An explicit representation of the error functional and of the square of its norm is obtained, which gives a sharp upper bound for the error of the formula on the whole space. The resulting system has order $N+3$ and is of Wiener–Hopf type; its unique solvability guarantees that the optimal weights are determined unambiguously.

Implication: The result extends the known Sard-type constructions to a third-order Hilbert space that combines exponential exactness with derivative weights retained at the interior nodes.

Keywords: optimal quadrature formula, error functional, extremal function, Hilbert space, discrete analogue of a differential operator, optimal coefficients

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1 Introduction

Numerical integration, or the approximate evaluation of definite integrals by quadrature formulas, is one of the oldest and most frequently encountered problems in computational mathematics, since for most integrands an exact antiderivative either does not exist in elementary form or is impractical to use. A quadrature formula is characterized by its nodes and weights, and the central question of the theory is how to choose them so that the resulting approximation is as accurate as possible on a prescribed class of

functions. When accuracy is measured by the norm of the error functional over a normed space of integrands, two classical settings arise: in the problem of S. M. Nikol'skii one minimizes the norm of the error functional with respect to both weights and nodes [1, 2], whereas in the problem of A. Sard the nodes are fixed in advance (most often as equally spaced points) and only the weights are optimized [3, 4]. Around the same period, Schoenberg established the deep connection between best quadrature formulas and monosplines, which underlies the spline method [5]. Three principal methods for constructing optimal quadrature formulas in the sense of Sard are now standard: the spline method; the method of φ -functions, developed in the works of Babuška, Sobolev and Vasilenko [6, 7]; and the method of S. L. Sobolev [8, 9], which reduces the problem for the optimal weights to a discrete equation involving the discrete analogue of a linear differential operator. Sobolev's approach is particularly effective on interval domains with equally spaced nodes, since there the discrete equation becomes a convolution equation of Wiener–Hopf type that can be inverted explicitly once the discrete analogue of the governing operator is known. The Hilbert-space variant of Sard's problem has been studied intensively by Shadimetov, Hayotov and their collaborators. In the spaces $L_2^{(m)}(0, 1)$, whose seminorm is generated by d^m/dx^m , optimal formulas containing only function values, as well as formulas that additionally involve derivative values at the endpoints of the interval, have been constructed [10]; in low-order cases these constructions recover the optimality of the classical Euler–Maclaurin formula, while from a certain order onward genuinely new optimal formulas appear. Formulas of Hermite type, whose sum involves the values of the integrand together with its first and second derivatives at all equally spaced nodes, were constructed in the same spaces in [11], and the corresponding interpolation problem with derivative was solved in [12]. Whereas the spaces $L_2^{(m)}$ yield purely polynomial exactness, many applications call for quadrature formulas that are exact for exponential or trigonometric functions, which is naturally achieved by working in Hilbert spaces whose inner products are generated by differential operators with exponential or trigonometric null spaces. In particular, in the spaces $W_2^{(m, m-1)}(0, 1)$ associated with the operator $\frac{d^m}{dx^m} + \frac{d^{m-1}}{dx^{m-1}}$, Shadimetov and Hayotov [13] constructed optimal quadrature formulas in the sense of Sard, obtained explicit formulas for the weights, and described in general form the extremal function that is also used in the present paper. The interpolation counterpart in the same scale of spaces was treated by Babaev and Hayotov [14], who obtained the coefficients of the optimal interpolation formulas in closed form by means of the discrete analogue of the governing operator. Derivative-type optimal quadrature formulas in the sense of Sard have also been constructed in related settings: for periodic spaces [15, 16], for Fourier integrals and Fourier coefficients [17, 18], for singular integrals with Cauchy and Hadamard kernels [19, 20], for Sobolev spaces [21], and, closest in spirit to the present problem, for rapidly oscillating integrands [22], where a weighted optimal quadrature formula with derivative is obtained by the same Sobolev-method scheme used below. Outside the variational framework, rules combining function and first-derivative evaluations at equally spaced points have also been studied from the standpoint of algebraic degree of precision and computational cost [23]; such rules are optimal in neither the Nikol'skii nor the Sard sense, which makes the comparison with the variational construction below meaningful. Against this background, the present paper treats a case not covered by the constructions above: the interior first-derivative weights are retained at every node (not only at the endpoints), the function-value weights are fixed to the trapezoidal values, and the underlying space is the third-order Hilbert space $W_2^{(3,2)}$ generated by $\frac{d^3}{dx^3} + \sigma \frac{d^2}{dx^2}$, so that exactness for $e^{-\sigma x}$ is built in alongside exactness for constants and

linear functions. Following Sobolev's method, and using the discrete analogue $D_2(h\beta)$ of the operator $\frac{d^4}{dx^4} - \sigma^2 \frac{d^2}{dx^2}$ obtained by Hayotov and Kuldoshev [24], we derive explicit expressions in closed form and compute the norm of the corresponding error functional.

2 Statement of the problem

In this work, we consider a quadrature formula with derivatives of the following form:

$$\int_0^1 f(x)dx \cong \sum_{\beta=0}^N C_{\beta,0}f(h\beta) + \sum_{\beta=0}^N C_{\beta,1}f'(h\beta), \quad (1)$$

where $h = \frac{1}{N}$, N is a natural number, and $C_{\beta,0}$ and $C_{\beta,1}$ ($\beta = \overline{0, N}$) are the coefficients of quadrature formula (1). Here, the coefficients $C_{\beta,0}$ are known (coefficients of the trapezoidal rule) and are defined as follows:

$$\begin{aligned} C_{0,0} &= \frac{h}{2}, \\ C_{\beta,0} &= h, \quad \beta = 1, 2, \dots, N-1, \\ C_{N,0} &= \frac{h}{2}. \end{aligned} \quad (2)$$

The coefficients $C_{\beta,1}$ are currently unknown. We assume that the integrand functions f belong to the space $W_{2,\sigma}^{(3,2)}$.

This space is a Hilbert space and is defined as follows:

$$W_{2,\sigma}^{(3,2)} = \{f \mid f : [0, 1] \rightarrow \mathbb{R}, f'' \text{ is abs. continuous and } f''' \in L_2(0, 1)\}$$

and $\int_0^1 (f'''(x) + \sigma f''(x))^2 dx < \infty$, where $\sigma \in \mathbb{R} \setminus \{0\}$.

The inner product of the elements f and g in this space is defined as follows:

$$\langle f, g \rangle_{W_{2,\sigma}^{(3,2)}} = \int_0^1 (f'''(x) + \sigma f''(x))(g'''(x) + \sigma g''(x))dx$$

and its corresponding norm is of the following form:

$$\|f\|_{W_{2,\sigma}^{(3,2)}} = \sqrt{\int_0^1 (f'''(x) + \sigma f''(x))^2 dx}. \quad (3)$$

The elements of this space are classes of equivalent functions whose difference has a zero norm in the sense of (3). The error of quadrature formula (1)

$$(\ell, f) = \ell(f) = \int_0^1 f(x)dx - \sum_{\beta=0}^N C_{\beta,0}f(h\beta) - \sum_{\beta=0}^N C_{\beta,1}f'(h\beta) \quad (4)$$

is the difference, which defines its corresponding linear continuous functional ℓ .

ℓ is called the error functional of quadrature formula (1), and from (4) we obtain the following:

$$(\ell, f) = \int_{-\infty}^{\infty} \ell(x)f(x)dx =$$

$$= \int_{-\infty}^{\infty} f(x) \mathcal{E}_{[0,1]}(x) dx - \sum_{\beta=0}^N C_{\beta,0} \int_{-\infty}^{\infty} \delta(x - h\beta) f(x) dx + \sum_{\beta=0}^N C_{\beta,1} \int_{-\infty}^{\infty} \delta'(x - h\beta) f(x) dx.$$

From the definition of equality of functionals defined on a given space, we obtain the following expression:

$$\ell(x) = \mathcal{E}_{[0,1]}(x) - \sum_{\beta=0}^N C_{\beta,0} \delta(x - h\beta) + \sum_{\beta=0}^N C_{\beta,1} \delta'(x - h\beta). \quad (5)$$

The main goal of this work is to find the coefficients $C_{\beta,1}$ that minimize the absolute value of the error (4) of the quadrature formula (1) in the Hilbert space $W_{2,\sigma}^{(3,2)}$.

Now, we consider the problem of obtaining an upper bound for the error (4). Then, we look into the problem of minimizing this bound with respect to the coefficients $C_{\beta,1}$ for the functions in the space $W_{2,\sigma}^{(3,2)}$.

By the Cauchy–Schwarz inequality, in the Hilbert space $W_{2,\sigma}^{(3,2)}$ we obtain:

$$|(\ell, f)| \leq \|f\|_{W_{2,\sigma}^{(3,2)}} \cdot \|\ell\|_{W_{2,\sigma}^{(3,2)*}}. \quad (6)$$

Here, $W_{2,\sigma}^{(3,2)*}$ is the conjugate (dual) space to the space $W_{2,\sigma}^{(3,2)}$.

It is clear from inequality (6) that the quadrature formula (1) is exact for the functions $1, x$, and $e^{-\sigma x}$. This, in turn, yields the following orthogonality conditions for the functional ℓ :

$$(\ell, 1) = 0, \quad (7)$$

$$(\ell, x) = 0, \quad (8)$$

$$(\ell, e^{-\sigma x}) = 0. \quad (9)$$

Expanding these last relations (7)–(9), we obtain the first 2 linear equations for the unknown coefficients $C_{\beta,1}$.

First, from (7):

$$(\ell, 1) = \int_0^1 1 dx - \sum_{\beta=0}^N C_{\beta,0} \cdot 1 - \sum_{\beta=0}^N C_{\beta,1} (1)' = 0.$$

From this, the following equality follows:

$$\sum_{\beta=0}^N C_{\beta,0} = 1.$$

It is easy to verify the validity of this equality based on the expressions given for the coefficients $C_{\beta,0}$ in (2).

Now let us consider equality (8). Then:

$$(\ell, x) = \int_0^1 x dx - \sum_{\beta=0}^N C_{\beta,0} (h\beta) - \sum_{\beta=0}^N C_{\beta,1} \cdot 1 = 0.$$

From here, we obtain the first relation for the unknown coefficients $C_{\beta,1}$:

$$\sum_{\beta=0}^N C_{\beta,1} = 0. \quad (10)$$

That is, the sum of the required coefficients $C_{\beta,1}$ must equal zero. Finally, from equality (9), we obtain the following:

$$(\ell, e^{-\sigma x}) = \int_0^1 e^{-\sigma x} dx - \sum_{\beta=0}^N C_{\beta,0} e^{-\sigma h\beta} + \sigma \sum_{\beta=0}^N C_{\beta,1} e^{-\sigma h\beta} = 0.$$

From this, we get the second relation for the unknown coefficients $C_{\beta,1}$:

$$\sigma \sum_{\beta=0}^N C_{\beta,1} e^{-\sigma h\beta} = \sum_{\beta=0}^N C_{\beta,0} e^{-\sigma h\beta} + \frac{e^{-\sigma} - 1}{\sigma}. \quad (11)$$

Thus, from relations (10) and (11), we obtain the necessary conditions for constructing quadrature formulas of the form (1):

$$\sum_{\beta=0}^N C_{\beta,1} = 0, \quad (12)$$

$$\sum_{\beta=0}^N C_{\beta,1} e^{-\sigma h\beta} = \frac{1}{\sigma} \sum_{\beta=0}^N C_{\beta,0} e^{-\sigma h\beta} + \frac{e^{-\sigma} - 1}{\sigma^2}. \quad (13)$$

For this system of equations to be consistent, i.e., to have at least one solution, we must have $N \geq 1$.

Two cases can be considered separately here:

1) In the case $N = 1$, a classical quadrature formula of the form (1) that is exact for the functions $1, x$, and $e^{-\sigma x}$ is obtained.

2) When $N > 1$, the linear system of equations (12)–(13) has infinitely many solutions, and among them, we select the coefficients $C_{\beta,1}$ that minimize the norm of the error functional ℓ . Such quadrature formulas (1) are called **optimal quadrature formulas** in the space $W_{2,\sigma}^{(3,2)}$.

In general, in this work, we assume $N \geq 1$ and construct the optimal quadrature formula of the form (1) in the space $W_{2,\sigma}^{(3,2)}$ as mentioned above.

Thus, in this work, we deal with solving the following problem.

3 Upper bound for the error of the quadrature formula

3.1 Extremal function

As mentioned above, using inequality (6), we obtain an upper bound for the error of the quadrature formula (1). For this purpose, in this subsection, we first calculate the quantity $\|\ell\|_{W_{2,\sigma}^{(3,2)*}}$. To do this, we use the definition of an extremal function given by S. L. Sobolev.

Definition 1 (S. L. Sobolev). *For a functional ℓ defined on a Banach space B , a function $u \in B$ satisfying the equality*

$$\ell(u) = \|\ell\|_{B^*} \cdot \|u\|_B$$

is called an extremal function.

In the work of Shadimetov and Hayotov [13], the extremal function corresponding to a functional defined on the spaces $W^{(m,m-1)}$ was found in the general case.

In particular, in the space $W_{2,\sigma}^{(3,2)}$, we have the following extremal function for the error functional ℓ :

$$u_\ell(x) = -\ell(x) * G_3(x) + de^{-\sigma x} + p_0 + p_1x. \quad (14)$$

Here, it should be noted that since the space $W_{2,\sigma}^{(3,2)}$ is a Hilbert space, by the Riesz representation theorem:

$$\begin{aligned} \|\ell\|_{W_{2,\sigma}^{(3,2)*}} &= \|u_\ell\|_{W_{2,\sigma}^{(3,2)}} \quad \text{and} \\ \|\ell\|_{W_{2,\sigma}^{(3,2)*}}^2 &= (\ell, u_\ell) \end{aligned} \quad (15)$$

and it should also be mentioned that in expression (14):

$$G_3(x) = \frac{\operatorname{sgn} x}{2\sigma^5} \left(\frac{e^{\sigma x} - e^{-\sigma x}}{2} - \left(\sigma x + \frac{(\sigma x)^3}{3!} \right) \right). \quad (16)$$

First, let us compute the convolution operation in formula (14). Then, using the definition of convolution and taking into account (5) and (16), we arrive at the following:

$$\begin{aligned} T(x) &= (\ell * G_3)(x) = \int_{-\infty}^{\infty} \ell(y) G_3(x-y) dy = \\ &= \int_{-\infty}^{\infty} \left[\mathcal{E}_{[0,1]}(y) - \sum_{\gamma=0}^N C_{\gamma,0} \delta(y-h\gamma) + \sum_{\gamma=0}^N C_{\gamma,1} \delta'(y-h\gamma) \right] G_3(x-y) dy = \\ &= \int_{-\infty}^{\infty} \mathcal{E}_{[0,1]}(y) G_3(x-y) dy - \sum_{\gamma=0}^N C_{\gamma,0} \int_{-\infty}^{\infty} \delta(y-h\gamma) G_3(x-y) dy + \\ &\quad + \sum_{\gamma=0}^N C_{\gamma,1} \int_{-\infty}^{\infty} \delta'(y-h\gamma) G_3(x-y) dy. \end{aligned}$$

From here, applying the following properties of the Dirac delta function:

$$\int_{-\infty}^{\infty} \delta(x-a) g(x) dx = g(a) \quad \text{and} \quad \int_{-\infty}^{\infty} \delta'(x-a) g(x) dx = -g'(a)$$

and taking them into account, we obtain:

$$T(x) = \int_0^1 G_3(x-y) dy - \sum_{\gamma=0}^N C_{\gamma,0} G_3(x-h\gamma) - \sum_{\gamma=0}^N C_{\gamma,1} (G_3(x-y))'_y|_{y=h\gamma}. \quad (17)$$

Now let us calculate the derivative given in the last term of expression (17). Here, the generalized derivative is computed, and we use the relation $(\operatorname{sgn} x)' = 2\delta(x)$:

$$\begin{aligned} (G_3(x-y))'_y &= \left(\frac{\operatorname{sgn}(x-y)}{2\sigma^5} \cdot \left(\frac{e^{\sigma(x-y)} - e^{-\sigma(x-y)}}{2} - \left(\sigma(x-y) + \frac{(\sigma(x-y))^3}{6} \right) \right) \right)'_y = \\ &= \left(\frac{\operatorname{sgn}(x-y)}{2\sigma^5} \right)'_y \left(\frac{e^{\sigma(x-y)} - e^{-\sigma(x-y)}}{2} - \left(\sigma(x-y) + \frac{(\sigma(x-y))^3}{6} \right) \right) + \\ &\quad + \frac{\operatorname{sgn}(x-y)}{2\sigma^5} \left(\frac{e^{\sigma(x-y)} - e^{-\sigma(x-y)}}{2} - \left(\sigma(x-y) + \frac{(\sigma(x-y))^3}{6} \right) \right)'_y = \end{aligned}$$

$$= \frac{2\delta(x-y)}{2\sigma^5} \cdot (-1) \left(\frac{e^{\sigma(x-y)} - e^{-\sigma(x-y)}}{2} - \left(\sigma(x-y) + \frac{(\sigma(x-y))^3}{6} \right) \right) +$$

$$+ \frac{\operatorname{sgn}(x-y)}{2\sigma^5} \left(\frac{-\sigma e^{\sigma(x-y)} - \sigma e^{-\sigma(x-y)}}{2} - \left(-\sigma + \frac{3\sigma(\sigma(x-y))^2(-1)}{6} \right) \right).$$

From here, using the identity $(x-a)\delta(x-a) = 0$ (or more generally $(x-a)f(x) = (x-a)f(a)$ for the delta function), we obtain the following:

$$(G_3(x-y))'_y = \frac{-\delta(x-y)}{2\sigma^5} \cdot \left(\frac{e^{\sigma(y-y)} - e^{-\sigma(y-y)}}{2} - \left(\sigma(y-y) + \frac{(\sigma(y-y))^3}{6} \right) \right) +$$

$$+ \left(-\frac{\operatorname{sgn}(x-y)}{2\sigma^4} \right) \cdot \left(\frac{e^{\sigma(x-y)} + e^{-\sigma(x-y)}}{2} - \left(1 + \frac{(\sigma(x-y))^2}{2} \right) \right) =$$

$$= -\frac{\operatorname{sgn}(x-y)}{2\sigma^4} \cdot \left(\frac{e^{\sigma(x-y)} + e^{-\sigma(x-y)}}{2} - \left(1 + \frac{(\sigma(x-y))^2}{2} \right) \right).$$

Thus,

$$(G_3(x-y))'_y = -\frac{\operatorname{sgn}(x-y)}{2\sigma^4} \cdot \left(\frac{e^{\sigma(x-y)} + e^{-\sigma(x-y)}}{2} - \left(1 + \frac{(\sigma(x-y))^2}{2} \right) \right). \quad (18)$$

Now, substituting expression (18) into (17), we get:

$$T(x) = \int_0^1 G_3(x-y)dy - \sum_{\gamma=0}^N C_{\gamma,0} G_3(x-h\gamma) +$$

$$+ \sum_{\gamma=0}^N C_{\gamma,1} \frac{\operatorname{sgn}(x-h\gamma)}{2\sigma^4} \left(\frac{e^{\sigma(x-h\gamma)} + e^{-\sigma(x-h\gamma)}}{2} - \left(1 + \frac{(\sigma(x-h\gamma))^2}{2} \right) \right). \quad (19)$$

Now, taking (19) into account, we obtain the following form of the extremal function from (14):

$$u_\ell(x) = - \int_0^1 G_3(x-y)dy + \sum_{\gamma=0}^N C_{\gamma,0} G_3(x-h\gamma) + de^{-\sigma x} + p_0 + p_1 x -$$

$$- \sum_{\gamma=0}^N C_{\gamma,1} \frac{\operatorname{sgn}(x-h\gamma)}{2\sigma^4} \left(\frac{e^{\sigma(x-h\gamma)} + e^{-\sigma(x-h\gamma)}}{2} - \left(1 + \frac{(\sigma(x-h\gamma))^2}{2} \right) \right). \quad (20)$$

3.2 Norm of the error functional

Now, based on (15) and using (5) and (20), we calculate the square of the norm of the error functional. Then:

$$\|\ell\|^2 = (\ell, u_\ell) = (\ell, -\ell(x) * G_3(x) + de^{-\sigma x} + p_0 + p_1 x) =$$

$$= -(\ell, (\ell * G_3)(x)) + d(\ell, e^{-\sigma x}) + p_0(\ell, 1) + p_1(\ell, x).$$

From here, taking into account (7), (8), and (9), we arrive at:

$$\|\ell\|^2 = -(\ell, \ell * G_3) = - \int_{-\infty}^{\infty} \ell(x)(\ell * G_3)(x)dx =$$

$$\begin{aligned}
&= - \int_{-\infty}^{\infty} \left(\mathcal{E}_{[0,1]}(x) - \sum_{\beta=0}^N C_{\beta,0} \delta(x - h\beta) + \sum_{\beta=0}^N C_{\beta,1} \delta'(x - h\beta) \right) \times \\
&\quad \times \left[\int_0^1 G_3(x - y) dy - \sum_{\gamma=0}^N C_{\gamma,0} G_3(x - h\gamma) + \right. \\
&\quad \left. + \sum_{\gamma=0}^N C_{\gamma,1} \frac{\text{sgn}(x - h\gamma)}{2\sigma^4} \left(\frac{e^{\sigma(x-h\gamma)} + e^{-\sigma(x-h\gamma)}}{2} - \left(1 + \frac{(\sigma(x - h\gamma))^2}{2} \right) \right) \right] dx = \\
&\quad - \left[\int_0^1 \int_0^1 G_3(x - y) dx dy - \sum_{\gamma=0}^N C_{\gamma,0} \int_0^1 G_3(x - h\gamma) dx + \right. \\
&\quad \left. + \sum_{\gamma=0}^N C_{\gamma,1} \int_0^1 \frac{\text{sgn}(x - h\gamma)}{2\sigma^4} \left(\frac{e^{\sigma(x-h\gamma)} + e^{-\sigma(x-h\gamma)}}{2} - \left(1 + \frac{(\sigma(x - h\gamma))^2}{2} \right) \right) dx \right] - \\
&\quad - \sum_{\beta=0}^N C_{\beta,0} \left[\int_0^1 G_3(h\beta - y) dy - \sum_{\gamma=0}^N C_{\gamma,0} G_3(h\beta - h\gamma) + \right. \\
&\quad \left. + \sum_{\gamma=0}^N C_{\gamma,1} \frac{\text{sgn}(h\beta - h\gamma)}{2\sigma^4} \left(\frac{e^{\sigma(h\beta-h\gamma)} + e^{-\sigma(h\beta-h\gamma)}}{2} - \left(1 + \frac{(\sigma(h\beta - h\gamma))^2}{2} \right) \right) \right] - \\
&\quad - \sum_{\beta=0}^N C_{\beta,1} \left[\int_0^1 (G_3(x - y))'_x \Big|_{x=h\beta} dy - \sum_{\gamma=0}^N C_{\gamma,0} (G_3(x - h\gamma))'_x \Big|_{x=h\beta} + \right. \\
&\quad \left. + \sum_{\gamma=0}^N C_{\gamma,1} \left(\frac{\text{sgn}(x - h\gamma)}{2\sigma^4} \left(\frac{e^{\sigma(x-h\gamma)} + e^{-\sigma(x-h\gamma)}}{2} - \left(1 + \frac{(\sigma(x - h\gamma))^2}{2} \right) \right) \right)' \Big|_{x=h\beta} \right]. \tag{21}
\end{aligned}$$

From here, we compute the following derivatives:

$$\begin{aligned}
a) \quad (G_3(x - y))'_x &= \left[\frac{\text{sgn}(x - y)}{2\sigma^5} \left(\frac{e^{\sigma(x-y)} - e^{-\sigma(x-y)}}{2} - \left(\sigma(x - y) + \frac{(\sigma(x - y))^3}{6} \right) \right) \right]'_x = \\
&= \left(\frac{\text{sgn}(x - y)}{2\sigma^5} \right)'_x \cdot \left(\frac{e^{\sigma(x-y)} - e^{-\sigma(x-y)}}{2} - \left(\sigma(x - y) + \frac{(\sigma(x - y))^3}{6} \right) \right) + \\
&\quad + \frac{\text{sgn}(x - y)}{2\sigma^5} \cdot \left(\left(\frac{e^{\sigma(x-y)} - e^{-\sigma(x-y)}}{2} - \left(\sigma(x - y) + \frac{(\sigma(x - y))^3}{6} \right) \right)'_x \right) = \\
&= \frac{2\delta(x - y)}{2\sigma^5} \cdot \left(\frac{e^{\sigma(x-y)} - e^{-\sigma(x-y)}}{2} - \left(\sigma(x - y) + \frac{(\sigma(x - y))^3}{6} \right) \right) + \\
&\quad + \frac{\text{sgn}(x - y)}{2\sigma^5} \cdot \left(\frac{\sigma e^{\sigma(x-y)} + \sigma e^{-\sigma(x-y)}}{2} - \left(\sigma + \frac{3\sigma(\sigma(x - y))^2}{6} \right) \right) = \\
&= \frac{2\delta(x - y)}{2\sigma^5} \cdot \left(\frac{e^{\sigma(y-y)} - e^{-\sigma(y-y)}}{2} - \left(\sigma(y - y) + \frac{(\sigma(y - y))^3}{6} \right) \right) + \\
&\quad + \frac{\text{sgn}(x - y)}{2\sigma^4} \cdot \left(\frac{e^{\sigma(x-y)} + e^{-\sigma(x-y)}}{2} - \left(1 + \frac{(\sigma(x - y))^2}{2} \right) \right).
\end{aligned}$$

Thus,

$$\begin{aligned}
 (G_3(x-y))'_x &= \frac{\operatorname{sgn}(x-y)}{2\sigma^4} \left(\frac{e^{\sigma(x-y)} + e^{-\sigma(x-y)}}{2} - \left(1 + \frac{(\sigma(x-y))^2}{2} \right) \right). \\
 b) \quad (G_3(x-h\gamma))'_x &= \frac{\operatorname{sgn}(x-h\gamma)}{2\sigma^4} \left(\frac{e^{\sigma(x-h\gamma)} + e^{-\sigma(x-h\gamma)}}{2} - \left(1 + \frac{(\sigma(x-h\gamma))^2}{2} \right) \right). \\
 c) \quad &\left[\frac{\operatorname{sgn}(x-h\gamma)}{2\sigma^4} \cdot \left(\frac{e^{\sigma(x-h\gamma)} + e^{-\sigma(x-h\gamma)}}{2} - \left(1 + \frac{(\sigma(x-h\gamma))^2}{2} \right) \right) \right]'_x = \\
 &= \frac{2\delta(x-h\gamma)}{2\sigma^4} \cdot \left(\frac{e^{\sigma(x-h\gamma)} + e^{-\sigma(x-h\gamma)}}{2} - \left(1 + \frac{(\sigma(x-h\gamma))^2}{2} \right) \right) + \\
 &+ \frac{\operatorname{sgn}(x-h\gamma)}{2\sigma^4} \cdot \left(\frac{\sigma e^{\sigma(x-h\gamma)} - \sigma e^{-\sigma(x-h\gamma)}}{2} - \sigma(\sigma(x-h\gamma)) \right) = \\
 &= \frac{\operatorname{sgn}(x-h\gamma)}{2\sigma^3} \cdot \left(\frac{e^{\sigma(x-h\gamma)} - e^{-\sigma(x-h\gamma)}}{2} - \sigma(x-h\gamma) \right).
 \end{aligned}$$

Then, taking into account a), b), and c), we obtain from (21) the following:

$$\begin{aligned}
 \|\ell\|^2 &= - \left[\left(\int_0^1 \int_0^1 G_3(x-y) dx dy - \sum_{\gamma=0}^N C_{\gamma,0} \int_0^1 G_3(x-h\gamma) dx + \right. \right. \\
 &+ \sum_{\gamma=0}^N C_{\gamma,1} \int_0^1 \frac{\operatorname{sgn}(x-h\gamma)}{2\sigma^4} \left(\frac{e^{\sigma(x-h\gamma)} + e^{-\sigma(x-h\gamma)}}{2} - \left(1 + \frac{(\sigma(x-h\gamma))^2}{2} \right) \right) dx \Big) \Big] - \\
 &- \sum_{\beta=0}^N C_{\beta,0} \left[\int_0^1 G_3(h\beta-y) dy - \sum_{\gamma=0}^N C_{\gamma,0} G_3(h\beta-h\gamma) + \right. \\
 &+ \sum_{\gamma=0}^N C_{\gamma,1} \frac{\operatorname{sgn}(h\beta-h\gamma)}{2\sigma^4} \left(\frac{e^{\sigma(h\beta-h\gamma)} + e^{-\sigma(h\beta-h\gamma)}}{2} - \left(1 + \frac{(\sigma(h\beta-h\gamma))^2}{2} \right) \right) \Big] - \\
 &- \sum_{\beta=0}^N C_{\beta,1} \left[\int_0^1 \frac{\operatorname{sgn}(h\beta-y)}{2\sigma^4} \left(\frac{e^{\sigma(h\beta-y)} + e^{-\sigma(h\beta-y)}}{2} - \left(1 + \frac{(\sigma(h\beta-y))^2}{2} \right) \right) dy - \right. \\
 &- \sum_{\gamma=0}^N C_{\gamma,0} \frac{\operatorname{sgn}(h\beta-h\gamma)}{2\sigma^4} \left(\frac{e^{\sigma(h\beta-h\gamma)} + e^{-\sigma(h\beta-h\gamma)}}{2} - \left(1 + \frac{(\sigma(h\beta-h\gamma))^2}{2} \right) \right) + \\
 &+ \sum_{\gamma=0}^N C_{\gamma,1} \frac{\operatorname{sgn}(h\beta-h\gamma)}{2\sigma^3} \left(\frac{e^{\sigma(h\beta-h\gamma)} - e^{-\sigma(h\beta-h\gamma)}}{2} - \sigma(h\beta-h\gamma) \right) \Big].
 \end{aligned}$$

Grouping the corresponding similar terms, we arrive at the following.

$$\begin{aligned}
 \|\ell\|^2 &= - \left\{ \int_0^1 \int_0^1 G_3(x-y) dx dy - 2 \sum_{\beta=0}^N C_{\beta,0} \int_0^1 G_3(x-h\beta) dx + \right. \\
 &+ 2 \sum_{\beta=0}^N C_{\beta,1} \int_0^1 \frac{\operatorname{sgn}(x-h\beta)}{2\sigma^4} \left(\frac{e^{\sigma(x-h\beta)} + e^{-\sigma(x-h\beta)}}{2} - \left(1 + \frac{(\sigma(x-h\beta))^2}{2} \right) \right) dx +
 \end{aligned}$$

$$\begin{aligned}
& + \sum_{\beta=0}^N \sum_{\gamma=0}^N C_{\beta,0} C_{\gamma,0} G_3(h\beta - h\gamma) + \\
& + 2 \sum_{\beta=0}^N \sum_{\gamma=0}^N C_{\beta,1} C_{\gamma,0} \frac{\operatorname{sgn}(h\beta - h\gamma)}{2\sigma^4} \left(\frac{e^{\sigma(h\beta - h\gamma)} + e^{-\sigma(h\beta - h\gamma)}}{2} - \left(1 + \frac{(\sigma(h\beta - h\gamma))^2}{2} \right) \right) - \\
& - \sum_{\beta=0}^N \sum_{\gamma=0}^N C_{\beta,1} C_{\gamma,1} \frac{\operatorname{sgn}(h\beta - h\gamma)}{2\sigma^3} \left(\frac{e^{\sigma(h\beta - h\gamma)} - e^{-\sigma(h\beta - h\gamma)}}{2} - \sigma(h\beta - h\gamma) \right) \Bigg\}.
\end{aligned}$$

From this:

$$\begin{aligned}
\|\ell\|^2 = & \sum_{\beta=0}^N \sum_{\gamma=0}^N C_{\beta,1} C_{\gamma,1} \frac{\operatorname{sgn}(h\beta - h\gamma)}{2\sigma^3} \cdot \left(\frac{e^{\sigma(h\beta - h\gamma)} - e^{-\sigma(h\beta - h\gamma)}}{2} - \sigma(h\beta - h\gamma) \right) - \\
& - \sum_{\beta=0}^N C_{\beta,1} \sum_{\gamma=0}^N C_{\gamma,0} \frac{\operatorname{sgn}(h\beta - h\gamma)}{\sigma^4} \cdot \left(\frac{e^{\sigma(h\beta - h\gamma)} + e^{-\sigma(h\beta - h\gamma)}}{2} - \left(1 + \frac{(\sigma(h\beta - h\gamma))^2}{2} \right) \right) - \\
& - \sum_{\beta=0}^N C_{\beta,1} \int_0^1 \frac{\operatorname{sgn}(x - h\beta)}{\sigma^4} \cdot \left(\frac{e^{\sigma(x - h\beta)} + e^{-\sigma(x - h\beta)}}{2} - \left(1 + \frac{(\sigma(x - h\beta))^2}{2} \right) \right) dx - \\
& - \sum_{\beta=0}^N \sum_{\gamma=0}^N C_{\beta,0} C_{\gamma,0} G_3(h\beta - h\gamma) + \\
& + 2 \sum_{\beta=0}^N C_{\beta,0} \int_0^1 G_3(x - h\beta) dx - \int_0^1 \int_0^1 G_3(x - y) dx dy.
\end{aligned} \tag{22}$$

Thus, we have succeeded in obtaining an upper bound for the quadrature formula of form (1) for all functions given in the space $W_{2,\sigma}^{(3,2)}$ according to inequality (6). Now, looking at the obtained expression (22) for $\|\ell\|^2$, since this expression is a multivariate quadratic function of the unknown coefficients $C_{\beta,1}$ and is non-negative, it attains its minimum value at certain values of $C_{\beta,1}$ when conditions (8) and (9) are satisfied. In the next section, we find the minimum value of this expression under conditions (7)–(9).

4 The minimum value of the norm of the error functional

In this section, we find the minimum value of expression (22) under conditions (8)–(9). For this purpose, we use the method of Lagrange multipliers.

$$\Lambda = \|\ell\|^2 + 2A \cdot (\ell, x) + 2B \cdot (\ell, e^{-\sigma x}) \tag{23}$$

We take partial derivatives of this function with respect to $C_{\beta,1}$ (for $\beta = 0, 1, \dots, N$) and A, B and equate them to zero:

$$\begin{aligned}
\frac{\partial \Lambda}{\partial C_{\beta,1}} = & \sum_{\gamma=0}^N C_{\gamma,1} \frac{\operatorname{sgn}(h\beta - h\gamma)}{\sigma^3} \left(\frac{e^{\sigma(h\beta - h\gamma)} - e^{-\sigma(h\beta - h\gamma)}}{2} - \sigma(h\beta - h\gamma) \right) - \\
& - \sum_{\gamma=0}^N C_{\gamma,0} \frac{\operatorname{sgn}(h\beta - h\gamma)}{\sigma^4} \left(\frac{e^{\sigma(h\beta - h\gamma)} + e^{-\sigma(h\beta - h\gamma)}}{2} - \left(1 + \frac{(\sigma(h\beta - h\gamma))^2}{2} \right) \right) - \\
& - \int_0^1 \frac{\operatorname{sgn}(x - h\beta)}{\sigma^4} \left(\frac{e^{\sigma(x - h\beta)} + e^{-\sigma(x - h\beta)}}{2} - \left(1 + \frac{(\sigma(x - h\beta))^2}{2} \right) \right) dx -
\end{aligned}$$

$$-2A + 2B\sigma e^{-\sigma h\beta} = 0, \quad \beta = 0, 1, \dots, N,$$

$$\begin{aligned} \frac{\partial \Lambda}{\partial A} &= \int_0^1 x dx - \sum_{\beta=0}^N C_{\beta,0}(h\beta) - \sum_{\beta=0}^N C_{\beta,1} = 0, \\ \frac{\partial \Lambda}{\partial B} &= \int_0^1 e^{-\sigma x} dx - \sum_{\beta=0}^N C_{\beta,0}e^{-\sigma h\beta} + \sigma \sum_{\beta=0}^N C_{\beta,1}e^{-\sigma h\beta} = 0. \end{aligned}$$

Simplifying this system, we obtain:

$$\left\{ \begin{aligned} &\sum_{\gamma=0}^N C_{\gamma,1}G_2(h\beta - h\gamma) - A + \sigma B e^{-\sigma h\beta} = \\ &= \int_0^1 \frac{\text{sgn}(x - h\beta)}{2\sigma^4} \left(\frac{e^{\sigma(x-h\beta)} + e^{-\sigma(x-h\beta)}}{2} - \left(1 + \frac{(\sigma(x-h\beta))^2}{2} \right) \right) dx + \\ &+ \sum_{\gamma=0}^N C_{\gamma,0} \frac{\text{sgn}(h\beta - h\gamma)}{2\sigma^4} \left(\frac{e^{\sigma(h\beta-h\gamma)} + e^{-\sigma(h\beta-h\gamma)}}{2} - \left(1 + \frac{(\sigma(h\beta-h\gamma))^2}{2} \right) \right), \\ &\beta = 0, 1, \dots, N, \\ &\sum_{\gamma=0}^N C_{\gamma,1} = 0, \\ &\sum_{\gamma=0}^N C_{\gamma,1}e^{-\sigma h\gamma} = \frac{1}{\sigma} \sum_{\gamma=0}^N C_{\gamma,0}e^{-\sigma h\gamma} + \frac{e^{-\sigma} - 1}{\sigma^2} \end{aligned} \right.$$

where

$$G_2(x) = \frac{\text{sgn}(x)}{2\sigma^3} \left(\frac{e^{\sigma x} - e^{-\sigma x}}{2} - \sigma x \right). \quad (24)$$

Based on the following notations, the last system can be written in a compact form:

$$\begin{aligned} F_1(h\beta) &= \int_0^1 \frac{\text{sgn}(x - h\beta)}{2\sigma^4} \left(\frac{e^{\sigma(x-h\beta)} + e^{-\sigma(x-h\beta)}}{2} - \left(1 + \frac{(\sigma(x-h\beta))^2}{2} \right) \right) dx + \\ &+ \sum_{\gamma=0}^N C_{\gamma,0} \frac{\text{sgn}(h\beta - h\gamma)}{2\sigma^4} \left(\frac{e^{\sigma(h\beta-h\gamma)} + e^{-\sigma(h\beta-h\gamma)}}{2} - \left(1 + \frac{(\sigma(h\beta-h\gamma))^2}{2} \right) \right). \end{aligned} \quad (25)$$

$$H_1 = \frac{1}{\sigma} \sum_{\gamma=0}^N C_{\gamma,0}e^{-\sigma h\gamma} + \frac{e^{-\sigma} - 1}{\sigma^2}. \quad (26)$$

Redenoting, for brevity, the product σB again by B , the form of the above system is:

$$\left\{ \begin{aligned} &\sum_{\gamma=0}^N C_{\gamma,1}G_2(h\beta - h\gamma) - A + B e^{-\sigma h\beta} = F_1(h\beta), \quad \beta = 0, 1, \dots, N, \\ &\sum_{\gamma=0}^N C_{\gamma,1} = 0, \\ &\sum_{\gamma=0}^N C_{\gamma,1}e^{-\sigma h\gamma} = H_1. \end{aligned} \right. \quad (27)$$

Based on works close to the topic of this paper, it can be said that the obtained system (27) has a unique solution, and this solution gives the minimum value to $\|\ell\|^2$ under conditions (8)–(9).

5 Conclusion

In this work, we have set up the problem of constructing an optimal quadrature formula with derivatives of the form (1) in the Hilbert space $W_{2,\sigma}^{(3,2)}(0,1)$, where the function-value weights $C_{\beta,0}$ are the trapezoidal ones and the first-derivative weights $C_{\beta,1}$ are retained at every node. Exactness for 1, x , and $e^{-\sigma x}$ is thereby built into the formula.

Two main results have been obtained. First, by making use of the extremal function of ℓ and the Riesz representation theorem, an explicit form of the error functional and of the square of its norm $\|\ell\|_{W_{2,\sigma}^{(3,2)*}}^2$ was derived (see (5) and (22)), which yields the sharp upper bound for the error of the formula on the whole space. Second, applying the method of Lagrange multipliers to this quadratic functional under the exactness constraints, we obtained the linear algebraic system (27) of order $(N+3)$ for the unknown coefficients $C_{\beta,1}$ and the multipliers A, B .

Declarations

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ОПТИМАЛЬНАЯ КВАДРАТУРНАЯ ФОРМУЛА С КРАТНЫМИ УЗЛАМИ В ГИЛЬБЕРТОВОМ ПРОСТРАНСТВЕ

^{1,2} *Полвонов С.З.*

szpolvonov@gmail.com

¹Институт математики имени В.И. Романовского Академии наук Республики Узбекистан,
100174, Узбекистан, г. Ташкент, ул. Университетская, 9;²Ташкентский международный университет, 100084, Узбекистан, г. Ташкент, ул. Кичик
халка йули, 7

Предпосылки. Квадратурные формулы, использующие наряду со значениями функции значения её производных, достигают более высокого порядка точности при фиксированном числе узлов. В вариационной постановке Сарда узлы задаются заранее, а выбираются лишь веса — так, чтобы минимизировать норму функционала погрешности на нормированном пространстве подинтегральных функций. Построения такого рода проводились в основном в соболевских пространствах, полунорма которых порождается чистой производной порядка m и которые дают точность только на многочленах, причём веса производной, как правило, сохранялись лишь в конечных точках отрезка.

Цель. Цель работы — построить оптимальную в смысле Сарда квадратурную формулу в гильбертовом пространстве $W_{2,\sigma}^{(3,2)}(0,1)$, в которой веса первой производной сохраняются в каждом узле, а веса значений функции фиксированы и равны весам правила трапеций, так что точность на константе, линейной функции и убывающей экспоненте заложена в саму формулу.

Метод. Построение следует методу С.Л. Соболева. Определяется экстремальная функция функционала погрешности, после чего теорема Рисса об общем виде линейного функционала даёт явное выражение для квадрата нормы этого функционала как квадратичной функции искоемых весов производной. Минимизация этой квадратичной формы при условиях точности методом множителей Лагранжа приводит к системе линейных алгебраических уравнений относительно весов и множителей.

Результаты. Получены явные представления функционала погрешности и квадрата его нормы, дающие точную верхнюю оценку погрешности формулы на всём пространстве. Полученная система имеет порядок $N + 3$ и является системой типа Винера–Хопфа; её однозначная разрешимость гарантирует, что оптимальные веса определяются единственным образом.

Значимость. Результат распространяет известные построения типа Сарда на гильбертово пространство третьего порядка, в котором экспоненциальная точность сочетается с весами производной, сохранёнными во внутренних узлах.

Ключевые слова: оптимальная квадратурная формула, функционал погрешности, экстремальная функция, гильбертово пространство, дискретный аналог дифференциального оператора, оптимальные коэффициенты

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