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OPTIMAL QUADRATURE FORMULA WITH DERIVATIVE

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Abstract

This article is devoted to the construction of optimal quadrature formulas with derivative in the space of differentiable functions using the Sobolev method. This quadrature formula consists of a linear combination of the values of the interval $[0,1]$ up to the second derivative of the function at all nodes. The error of the quadrature formulas is estimated by the norm of the error function. We obtain the optimal quadrature formula by minimizing the norm of the error functional by the coefficients of the quadrature formula with derivative. Numerical examples are provided to demonstrate the effectiveness and accuracy of the work presented.

Math. Subject Classification: 65D30, 65D32
Key Words and Phrases: Sobolev space, quadrature formula, error functional, optimal coefficients.

1. Introduction

Optimal quadrature formulas with derivative are methods of approximate calculation of definite integrals. They are necessary for calculating the integrals when an antiderivative of the functions under the integral cannot be expressed by elementary functions or the integrand exists only at discrete points. The use of formulas with a high level of algebraic accuracy in the integration of non-smooth functions does not lead to the good results. Therefore, it is important to construct optimal quadrature formulas with derivatives in the space of differentiable functions and estimate their errors. In this work, optimal quadrature formulas with derivatives are obtained based on the variational approach for the approximate calculation of definite integrals and numerical solutions of integral equations using the values of the given function up to the second order derivative at the nodes.

We consider the following quadrature formula

$$\int_0^1 u(x)dx \cong \sum_{\beta=0}^{N} C_0[\beta]\, u[\beta] + \frac{h^2}{12}(u'[0]-u'[1]) + \sum_{\beta=0}^{N} C_1[\beta]\, u''[\beta] \tag{1}$$

the difference below is the error of the quadrature formula

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$$(\ell_N, u) = \int_0^1 u(x)dx - \sum_{\beta=0}^{N} C_0[\beta]\, u[\beta] - \frac{h^2}{12}(u'[0] - u'[1]) - \sum_{\beta=0}^{N} C_1[\beta]\, u''[\beta]$$

with error functional

$$\ell_N(x) = \varepsilon_{[0,1]}(x) - \sum_{\beta=0}^{N} C_0\,[\beta]\delta(x-\beta) + \frac{h^2}{12}\big(\delta'(x) - \delta'(x-1)\big)$$
$$- \sum_{\beta=0}^{N} C_1\,[\beta]\delta''(x-\beta) \quad (2)$$

where $\varepsilon_{[0,1]}(x)$ is the indicator of the interval $[0,1]$, $\delta(x)$ is the Dirac's delta-function, $C_0[\beta] = \begin{cases} \frac{h}{2}, & \beta = 0, N, \\ h, & \beta = \overline{1, N-1}, \end{cases}$ $[\beta] = h\beta$, $h = \frac{1}{N}$, N is a natural number.

According to the definition of the functional norm

$$\left\| \ell_N \middle| L_2^{(m)^*} \right\| = \sup_{\|u|L_2^{(m)}\| \neq 0} \frac{|(\ell_N, u)|}{\|u|L_2^{(m)}\|}$$

from this, we get the Cauchy-Schwarz inequality

$$|(\ell_N, u| \leq \| u \Big| L_2^{(m)} \| \cdot \| \ell_N \Big| L_2^{(m)^*} \|$$

As it can be seen from this inequality, the error of the quadrature formula with derivative (1) is estimated by the product of the norm of the error functional $\ell_N(x)$ obtained from the conjugate space $L_2^{(m)^*}$ and the norm of the function u obtained from the space $L_2^{(m)}(0,1)$. Since the error function ℓ_N is defined in space $L_2^{(m)}(0,1)$, it satisfies the following conditions

$$(\ell_N, x^\alpha) = 0, \quad \alpha = 0,1,2,\ldots, m-1. \quad (3)$$

The norm of the error function (2) depends on $C_1[\beta]$ coefficients, and we minimize the norm of the error function by $C_1[\beta]$ coefficients. In order to construct the optimal quadrature formula with derivatives in the form (1), we need to solve the following problems [1,2] .

Problem 1. *Finding the general view of the error functional norm (2) of the quadrature formula with derivatives of the form (1) in* $L_2^{(m)*}(0,1)$ *space.*

Problem 2. *To find the coefficients that give the minimum to the norm of the error functional.*

2. Main results

To solve **Problem 1**, we use the Riess theorem [3]. The norm of the error function can be written as follows [4,5]

$$\|\ell_N\|^2 = (\ell_N, U_\ell) = \Big(\ell_N(x), \big((-1)^m \ell_N(x) * G_{m-2}(x) + P_{m-1}(x)\big)\Big)$$

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where

$$U_\ell(x) = (-1)^m \ell_N(x) * G_{m-2}(x) + P_{m-1}(x),$$
$$G_{m-2}(x) = \frac{|x|^{2m-5}}{2 \cdot (2m-5)!}$$

The following is true [6].

Theorem 1. *An overview of the norm of the error functional (2) corresponding to the derivative quadrature formula (1) is as follows*

$$\|\ell_N\|^2 = (-1)^m \Big[\sum_{\beta=0}^N C_1[\beta] \sum_{\gamma=0}^N C_1[\gamma] \frac{|[\beta]-[\gamma]|^{2m-5}}{2(2m-5)!} - 2\sum_{\beta=0}^N C_1[\beta] \int_0^1 \frac{|x-[\beta]|^{2m-3}}{2(2m-3)!} dx$$
$$- \frac{h^2}{6} \sum_{\beta=0}^N C_1[\beta] \left[\frac{([\beta]^{2m-4} + (1-[\beta])^{2m-4}}{2(2m-4)!}\right] + 2\sum_{\beta=0}^N C_0[\beta] \sum_{\gamma=0}^N C_1[\gamma] \frac{|[\beta]-[\gamma]|^{2m-3}}{2(2m-3)!}$$
$$- \frac{h^2}{6} \sum_{\beta=0}^N C_0[\beta] \left[\frac{[\beta]^{2m-2} + (1-[\beta])^{2m-2}}{2(2m-2)!}\right] - 2\sum_{\beta=0}^N C_0[\beta] \int_0^1 \frac{|x-[\beta]|^{2m-1}}{2(2m-1)!} dx$$
$$+ \sum_{\beta=0}^N C_0[\beta] \sum_{\gamma=0}^N C_0[\gamma] \frac{|[\beta]-[\gamma]|^{2m-1}}{2(2m-1)!} + \frac{h^2}{6(2m-1)!} + \frac{1}{(2m+1)!} + \frac{h^4}{144(2m-3)!}\Big].$$

Theorem 2. *For the coefficients of the optimal quadrature formula (1) in* $L_2^{(4)}(0,1)$ *space the following equalities hold* $C_1[0] = C_1[N] = ah\frac{q-q^N}{q-1}$, $C_1[\beta] = ah\left(q^\beta + q^{N-\beta}\right)$, $\beta = \overline{1, N-1}$, *where* $a = \frac{h^2}{120(1+q^N)}$, $q = \sqrt{3} - 2$.

Proof. To determine the optimal coefficients, we employ the method of Lagrange multipliers. In this context, based on the conditions (3), we formulate the following Lagrange function

$$\Phi(C_1[\beta], \lambda_\alpha) = \|\ell_N\|^2 + (-1)^m(\ell_N, x^\alpha), \quad \alpha = 0,1 \tag{4}$$

From the (4), by equating the partial derivatives for the unknown constants $C_1[\beta]$ and λ_α to zero, we get the following system

$$\sum_{\gamma=0}^N C_1[\gamma]\, G_2([\beta]-[\gamma]) + P_1[\beta] = f_4[\beta], \qquad \beta = \overline{0, N}, \tag{5}$$

$$\sum_{\gamma=0}^N C_1[\gamma] = 0, \qquad \sum_{\gamma=0}^N C_1[\gamma]\,[\beta] = 0 \tag{6}$$

To get an analytical solution for these equations, we use discrete analogue of the differential operator $\frac{d^4}{dx^4}$ [7], when $\beta < 0$ and $\beta > N$ for $C_1[\beta] = 0$. Then, we write equation (5) in the form of convolution

$$C_1[\gamma] * G_2[\beta] + P_1[\beta] = f[\beta], \qquad \beta = \overline{0, N} \tag{7}$$

$$f[\beta] = \frac{h^4}{1440}\left[[\beta]^2 - [\beta] + \frac{1}{2}\right] + \frac{h^6}{30240}.$$

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We will use the $u[\beta]$ notation presented on the left-hand side of equation (7). This means that to find the optimal coefficients $C_1\,[\beta]$ it is necessary to determine the values of the function

$u(h\beta)$ for all integer values β. $u[\beta]=f[\beta]$ for $\beta=0,\,1,\,\ldots,\,N$. We can find the values $C_1[\beta]$ for $\beta=1,2,\ldots N-1$

$$C_1[\beta]=hD_2[\beta]*u[\beta]=h\left[aq^{\beta}+bq^{N-\beta}\right] \tag{8}$$

where

$$a=\sqrt{3}h^4\sum_{\gamma=1}^{\infty}q^{\gamma}(Q_1^{-}[-\gamma]-f[-\gamma]),$$

$$b=\sqrt{3}h^4\sum_{\gamma=1}^{\infty}q^{\gamma}(Q_1^{+}[N+\gamma]-f[N+\gamma]).$$

We need find a and b. To do this, we calculate on the left side of (5) the following sum

$$S[\beta]=C_1[0]\tfrac{[\beta]^3}{6}+S_1[\beta]-S_2[\beta] \tag{9}$$

$$S_1[\beta]=\sum_{\gamma=1}^{\beta-1}C_1[\gamma]\frac{([\beta]-[\gamma])^3}{6},\quad S_2[\beta]=\sum_{\gamma=0}^{N}C_1[\gamma]\frac{([\beta]-[\gamma])^3}{12}.$$

Calculate $S_1(h\beta)$ [8]

$$S_1(h\beta)=-\textstyle\sum_{j=0}^{3}\frac{(h\beta)^{3-j}}{j!(3-j)!}h^{j+1}\left[\frac{aq}{q-1}\sum_{i=0}^{3}\left(\frac{1}{q-1}\right)^i\Delta^i0^j-\frac{bq^N}{1-q}\sum_{i=0}^{3}\left(\frac{q}{1-q}\right)^i\Delta^i0^j\right] \tag{10}$$

Calculate $S_2(h\beta)$

$$S_2(h\beta)=\tfrac{h\beta}{4}\textstyle\sum_{\gamma=0}^{N}K_1[\gamma](h\gamma)^2-\tfrac{1}{12}\sum_{\gamma=0}^{N}K_1[\gamma](h\gamma)^3 \tag{11}$$

We substitute equalities (10) and (11) into (9), equate the corresponding powers $[\beta]$

$$C_1[0]=h\tfrac{aq-bq^N}{q-1},\qquad \tfrac{aq+bq^{N+1}}{(q-1)^2}=\tfrac{B_4h^2}{24} \tag{12}$$

In equality (6) using (12), we find the form $C_1[N]$

$$C_1[N]=h\frac{bq-aq^N}{q-1}.$$

As stated above, we can expand equality (7) using (10), (11) and (12)

$$h^2\sum_{i=0}^{1}\frac{aq^i+bq^{N+1}(-1)^{N+1}}{(1-q)^{i+1}}\Delta^i0^1+h\frac{aq^N}{1-q}$$

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$$-\sum_{p=0}^{1}\frac{h^{p+1}}{p!(1-p)!}\sum_{i=0}^{1}\frac{aq^{N+i}+bq(-1)^{N+1}}{(1-q)^{i+1}}\Delta^{i}0^{p}+h\frac{bq}{q-1}=0 \tag{13}$$

From equality (13) we equate the corresponding powers h

$$\frac{aq+bq^{N+1}}{(1-q)^2}=\frac{aq^{N+1}+bq}{(1-q)^2} \tag{14}$$

we find a and b, from (12) and (14)

$$a=b=\frac{h^2}{120(1+q^N)}$$

Theorem 2 is completely proved. □

3. Numerical results

For numerical solution of definite integrals, optimal quadrature formulas with derivatives were constructed using the Sobolev method in [9,10]. In this work, we constructed an optimal quadrature formula using the first and second derivatives of the function at the nodes.

In Table 1, for the approximate computation of definite integrals using $N=10$ nodal points, the error of Simpson's rule **(Error1)** and the error of the derivative-based quadrature formulas constructed in this work **(Error2)** are defined. The numerical computation errors for the definite integrals of the following five functions are provided $I=\int_0^1 u(x)dx$

a) $u(x)=e^{-\cos x}+2\sin x$ b) $u(x)=\ln(1+x^2)+\sqrt{1+x^3}$

c) $u(x)=\cos 2x-\frac{1}{1+x^2}$ d) $u(x)=e^{x^2}$

Table 1. Errors

Error	1-example	2-example	3-example	4-example
Error1	8.75×10^{-7}	2.70×10^{-6}	4.07×10^{-6}	2.96×10^{-5}
Error2	1.05×10^{-8}	4.12×10^{-8}	4.77×10^{-8}	8.36×10^{-7}

In Table 2, the error of the derived formula from [11] **(I-MSONC4)** and the error of the formula constructed in this work **(Error2)** are numerically analyzed using the following five functions

a) $f(x)=e^{-x}$ b) $f(x)=\frac{1}{1+x}$

c) $f(x)=\sqrt{1+x^2}$ d) $f(x)=\frac{\ln(1+x)}{1+x^2}$

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Table 2. Errors

Error	**1-example**	**2-example**	**3-example**	**4-example**
I - MSONC4	9.60×10^{-4}	7.96×10^{-3}	1.27×10^{-3}	1.42×10^{-2}
Error2	8.50×10^{-4}	5.64×10^{-3}	3.87×10^{-4}	7.53×10^{-3}

In Table 3, the square of the error functional norm of the derivative-based optimal quadrature formula constructed in [12] **(Error1)** and the square of the error functional norm of the optimal quadrature formula with derivative in this work **(Error2)** are numerically analyzed at $N = 10,\ \ N = 100,\ N = 500,\ N = 1000$ node points

Table 3. Errors

$\|\ell_N\|^2$	**N=10**	**N=100**	**N=500**	**N=1000**
Error1	9.93×10^{-15}	8.42×10^{-23}	2.12×10^{-28}	2.29×10^{-31}
Error2	9.38×10^{-15}	8.37×10^{-23}	2.02×10^{-28}	1.77×10^{-31}

4. Conclusion

In conclusion, this research is related to the construction of optimal quadrature formulas with derivatives using the second-order derivative of a function at nodal points for the approximate calculation of definite integrals and the numerical solution of integral equations in the $L_2^{(m)}(0,1)$ space. As a result of the study, the square of the norm of the error functional of the derived optimal quadrature formulas was determined. The system of algebraic equations was derived to minimize this norm through coefficients. By solving the system of equations, the optimal coefficients were obtained. The efficiency and effectiveness of the constructed formula in the numerical solution of definite integrals are demonstrated in the tables.

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