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THE WEIGHTED OPTIMAL QUADRATURE FORMULA WITH DERIVATIVES IN THE HILBERT SPACE

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In the present article, the problem of constructing the optimal quadrature formula in the sense of Sard is discussed for numerical integration of the weighted integrals in the Hilbert space of real-valued functions. Initially, the norm of the error functional is found using the extremal function of the error functional of the quadrature formula. Since the error functional is defined on the Hilbert space, the quadrature formula that we are constructing is exact for zeros of this space, that is, we have the conditions that the influence of the error functional on these functions is equal to zero. Then, the Lagrange function is constructed to find the conditional extremum of the error functional norm. Thereby, a system of linear equations is obtained for the coefficients of the optimal quadrature formula.

Keywords: quadrature formula with derivatives, extremal function, error functional, optimal coefficient, Lagrange function.

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1 Introduction

Quadrature formulas are used to estimate definite integrals and are essential for numerically solving differential and integral equations. These formulas involve nodes and coefficients, and various methods are available to construct them. One such method is the variational approach, which is based on the principles and functionals of variational calculus. The primary objective of this approach is to identify the nodes and weights that minimize or maximize a specific functional related to the estimation of the integral. Several studies have been conducted on this approach [6, 7, 17, 23].

In general, quadrature rules can be used to compute integrals with a weight function, i.e., integrals of the form

$$\int_a^b p(x)f(x)\mathrm{d}x \approx \sum_{\beta=0}^{N} C_\beta f(x_\beta),$$

where $p(x)$ is a nonnegative weight function defined on the interval (a, b). By including the effect of $p(x)$ in the quadrature weights and points, one can obtain an accurate approximation of the integral even for integrands that behave poorly, such as singular, discontinuous, or highly oscillatory functions.

The main advantage of using weighted quadrature rules is that they can handle the "bad"behaviour of $p(x)$, which is known and can be factored out into the weight function. By designing a quadrature rule with $p(x)$ taken into account, one can achieve fast convergence, provided that the remaining factor $f(x)$ is smooth. Moreover, the same rule can be used for different $f(x)$ as long as $p(x)$ remains the same.

A large number of scientific studies have been devoted to the construction of optimal quadrature formulas with weight $p(x) = e^{2\pi i\omega x}$ (highly oscillatory) in the sense of Sard and their application. Previous studies [3, 9, 12, 13, 15, 16, 21] have focused on the construction of optimal quadrature formulas for the numerical integration of Fourier integrals in the Hilbert and Sobolev spaces and applied these results to computed tomography problems.

Even in cases where $p(x)$ is weakly singular [5, 8, 10, 11, 22] and singular [1, 2, 18], optimal quadrature formulas were constructed in different Hilbert and Sobolev spaces.

2 Auxiliary results

In [19], the following weighted optimal quadrature formulas with derivatives were constructed in $L_2^{(m)}(0,1)$ space:

$$\int_0^1 p(x)\varphi(x)\mathrm{d}x \cong \sum_{\beta=0}^{N}\sum_{\alpha=0}^{m-1} C_{\beta,\alpha}\varphi^{(\alpha)}(x_\beta), \tag{1}$$

where $x_\beta = h\beta \in [0,1]$, $h = \frac{1}{N}$, N is the number of quadrature nodes, $p(x)$ is the weight function, and a function $\varphi(x)$ belongs to the Sobolev space

$$L_2^{(m)}(0,1) = \{\varphi : [0,1] \to \mathbb{R} \mid \varphi^{(m-1)} \text{ are abs. cont. and } \varphi^{(m)} \in L_2(0,1)\}.$$

A sequential optimization method is used to construct the optimal quadrature formula of the form (1). It is based on the following algorithm:

Initially, when $m = 1$, the optimal quadrature formula exact for a constant function is constructed in the following form:

$$\int_0^1 p(x)\varphi(x)\mathrm{d}x \cong \sum_{\beta=0}^{N} C_{\beta,0}\varphi(x_\beta). \tag{2}$$

Then, for the case $m = 2$, construct an optimal quadrature formula exact for functions 1 and x,

$$\int_0^1 p(x)\varphi(x)\mathrm{d}x \cong \sum_{\beta=0}^{N} C_{\beta,0}\varphi(x_\beta) + \sum_{\beta=0}^{N} C_{\beta,1}\varphi'(x_\beta). \tag{3}$$

Here using the coefficients of quadrature formula (2) as coefficients $C_{\beta,0}$, and quadrature formula (3) is optimized according to coefficients $C_{\beta,1}$. Continuing by this manner, i.e. putting the obtained optimal coefficients $C_{\beta,0}$, $C_{\beta,1}$, …, $C_{\beta,m-2}$ to the quadrature formulas (1) and optimizing this quadrature formulas by coefficients $C_{\beta,m-1}$ in $L_2^{(m)}(0,1)$ space we have optimal quadrature formula exact for functions 1, x, x^2, …, x^{m-1}.

Theorem 1. (Theorem 3.1. of [19]) *The optimal coefficients for the quadrature formulas of the form (1) in the Sobolev space $L_2^{(m)}(0,1)$ are defined as follows:*

$$C_{0,k} = \frac{p_k}{2} + h^{-1}(-1)^k\left[F_k(h) - F_k(0)\right], \tag{4}$$

$$C_{\beta,k} = h^{-1}(-1)^k\left[F_k(h(\beta-1)) + 2F_k(h\beta) + F_k(h(\beta+1))\right], \quad \beta = 1,\dots,N-1, \tag{5}$$

$$C_{N,k} = \frac{p_k}{2} + h^{-1}(-1)^k \left[F_k(1-h) - F_k(1)\right]. \tag{6}$$

Here $k = m-1$,

$$F_k(h\beta) = f_k(h\beta) - \sum_{\gamma=0}^{N}\sum_{\alpha=0}^{k-1}(-1)^\alpha C_{\gamma,\alpha}\frac{(h\beta-h\gamma)^{k-\alpha+1}\operatorname{sign}(h\beta-h\gamma)}{2(k-\alpha+1)!},$$

$$f_k(h\beta) = (-1)^k\int_0^1 p(x)\frac{(x-h\beta)^{k+1}\operatorname{sign}(x-h\beta)}{2(k+1)!}dx,$$

$$p_k(h\beta) = \frac{g_k}{k!} - \sum_{\gamma=0}^{N}\sum_{\alpha=0}^{k-1}C_{\gamma,\alpha}\frac{(h\gamma)^{k-\alpha}}{(k-\alpha)!},$$

$$g_k = \int_0^1 p(x)x^k dx.$$

3 Statement of the problem

To achieve high accuracy, we are developing an optimal quadrature formula that includes exactness for function e^{-x}.

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

$$\int_0^1 p(x)\varphi(x)dx \cong \sum_{\beta=0}^{N}\sum_{\alpha=0}^{m-2}C^{(L)}_{\beta,\alpha}\varphi^{(\alpha)}(x_\beta) + \sum_{\beta=0}^{N}C^{(W)}_{\beta,m-1}\varphi^{(m-1)}(x_\beta), \tag{7}$$

where, $p(x)$ is the weight function, x_β are nodes of quadrature formula (7) and function φ belongs to the linear space $W_2^{(m,m-1)}(0,1)$ which is defined as (see [3, 4])

$$W_2^{(m,m-1)}(0,1) = \{\varphi : (0,1) \to \mathbb{R} | \varphi^{(m-1)} \text{ is abs. cont, and } \varphi^{(m)} \in L_2(0,1)\}.$$

The following difference is called the error of the quadrature formula (7)

$$(\ell,\varphi) = \int_0^1 p(x)\varphi(x)dx - \sum_{\beta=0}^{N}\sum_{\alpha=0}^{m-2}C^{(L)}_{\beta,\alpha}\varphi^{(\alpha)}(x_\beta) - \sum_{\beta=0}^{N}C^{(W)}_{\beta,m-1}\varphi^{(m-1)}(x_\beta), \tag{8}$$

and the following error functional corresponds to it

$$\ell(x) = \varepsilon_{[0,1]}(x)p(x) - \sum_{\beta=0}^{N}\sum_{\alpha=0}^{m-2}(-1)^\alpha C^{(L)}_{\beta,\alpha}\delta^{(\alpha)}(x-x_\beta) - (-1)^{m-1}\sum_{\beta=0}^{N}C^{(W)}_{\beta,m-1}\delta^{(m-1)}(x-x_\beta). \tag{9}$$

Here, $C^{(L)}_{\beta,\alpha}$ are known coefficients of optimal quadrature formula (1), $C^{(W)}_{\beta,m-1}$ are the unknown coefficients of quadrature formula (7), $\varepsilon_{[0,1]}(x)$ is the characteristic function of the interval $[0,1]$, and $\delta(x)$ is Dirac's delta-function.

The inner product of two functions $\varphi(x)$ and $\psi(x)$ in the space $W_2^{(m,m-1)}(0,1)$ is defined as

$$\langle\varphi,\psi\rangle = \int_0^1 (\varphi^{(m)}(x) + \varphi^{(m-1)}(x))(\psi^{(m)}(x) + \psi^{(m-1)}(x))dx.$$

And norm of the function in this space is determined as

$$\|\varphi\|_{W_2^{(m,m-1)}} = \sqrt{\langle\varphi,\varphi\rangle}.$$

The error of the quadrature formula is a linear functional in $W_2^{(m,m-1)*}(0,1)$, where $W_2^{(m,m-1)*}(0,1)$ is the dual space to the space $W_2^{(m,m-1)}(0,1)$.

The quadrature formula of the form (7) was constructed in work [14] when $p(x)=1$ and $m=2$.

It is natural to evaluate the quality of the quadrature formula (7) using the maximum error of this formula on the unit ball of the Hilbert space $W_2^{(m,m-1)}(0,1)$, that is, using the norm of the functional

$$\|\ell\|_{W_2^{(m,m-1)*}} = \sup_{\|\varphi\|_{W_2^{(m,m-1)}}=1} |(\ell,\varphi)|.$$

Obviously, the norm of the error functional depends on $C^{(W)}_{\beta,m-1}$ coefficients and x_β nodes.

If

$$\|\mathring{\ell}\|_{W_2^{(m,m-1)*}} = \inf_{C^{(W)}_{\beta,m-1},x_\beta} \|\ell\|_{W_2^{(m,m-1)*}}$$

then the functional $\mathring{\ell}$ is said to correspond to *the optimal quadrature formula* in $W_2^{(m,m-1)}(0,1)$.

Problem above in such a general formulation is quite difficult. Minimizing the norm of the error functional with respect to the coefficients $C^{(W)}_{\beta,m-1}$ is a linear problem, and with respect to the nodes x_β it is actually non-linear, complicated problem, therefore, for simplicity, we consider this problem with fixed nodes x_β (for instance, $x_\beta=h\beta$).

The main problem, in this work, is as follows.

Problem 1. Find the coefficients $\mathring{C}^{(W)}_{\beta,m-1}$ that give minimum value to $\|\ell\|_{W_2^{(m,m-1)*}}$, and calculate

$$\left\|\mathring{\ell}\right\|_{W_2^{(m,m-1)*}} = \inf_{C^{(W)}_{\beta,m-1}} \|\ell\|_{W_2^{(m,m-1)*}}.$$

4 The norm of error functional

For solving this problem, firstly, we must find the norm of the error functional. For this we need an extremal function of the error functional ℓ. General form of the extremal function in $W_2^{(m,m-1)}(0,1)$ space was found in works [4] and [20]. In particular, we get the following

$$\|\ell\|^2_{W_2^{(m,m-1)*}} = (\ell,\psi_\ell) = \int_{-\infty}^{\infty} \ell(x)\psi_\ell(x)dx, \tag{10}$$

here ψ_ℓ is the extremal function and it is defined as follows

$$\psi_\ell(x) = (-1)^m \ell(x) * G_m(x) + P_{m-2}(x) + de^{-x}, \tag{11}$$

herein

$$G_m(x) = \frac{\operatorname{sign}(x)}{2}\left(\frac{e^x-e^{-x}}{2} - \sum_{k=1}^{m-1}\frac{x^{2k-1}}{(2k-1)!}\right).$$

Using (11) from relation (10) we get the following

$$\|\ell\|^2_{W_2^{(m,m-1)*}} = (\ell,\psi_\ell) = \int_{-\infty}^{\infty} \ell(x)\left((-1)^m\ell(x)*G_m(x)+P_{m-2}(x)+de^{-x}\right)dx. \tag{12}$$

It should be noted that since the error functional $\ell(x)$ is defined on the space $W_2^{(m,m-1)}$, it satisfies the following conditions

$$\left(\ell, e^{-x}\right) = 0, \tag{13}$$

$$\left(\ell, x^k\right) = 0, \quad k = 0, 1, \ldots, m-2. \tag{14}$$

The equalities (13) and (14) mean that the quadrature formula (7) is exact for the function e^{-x} and for any polynomial of degree $\leqslant m-2$.

Then, from equality (12), taking into account the expressions (13) and (14), we have the following

$$\|\ell\|^2_{W_2^{(m,m-1)*}} = (-1)^m \int_{-\infty}^{\infty} \ell(x) \left(\ell(x) * G_m(x)\right) dx \tag{15}$$

Firstly, we calculate $\ell(x) * G_m(x)$ from the last equality:

$$\begin{aligned}\ell(x) * G_m(x) &= \int_0^1 p(y) G_m(x-y) dy - \sum_{\gamma=0}^{N} \sum_{\alpha=0}^{m-2} (-1)^\alpha C^{(L)}_{\gamma,\alpha} G_m^{(\alpha)}(x-h\gamma) - \\ &\quad -(-1)^{m-1} \sum_{\gamma=0}^{N} C^{(W)}_{\gamma,m-1} G_m^{(m-1)}(x-h\gamma).\end{aligned}$$

Now, from equality (15), taking into account the above expression and (9), we get

$$\begin{aligned}\|\ell\|^2_{W_2^{(m,m-1)*}} &= (-1)^m \int_{-\infty}^{\infty} \Bigg(\varepsilon_{[0,1]}(x) p(x) - \sum_{\beta=0}^{N} \sum_{\alpha=0}^{m-2} (-1)^\alpha C^{(L)}_{\beta,\alpha} \delta^{(\alpha)}(x-h\beta) - \\ &\quad -(-1)^{m-1} \sum_{\beta=0}^{N} C^{(W)}_{\beta,m-1} \delta^{(m-1)}(x-h\beta) \Bigg) \times \\ &\quad \times \Bigg(\int_0^1 p(y) G_m(x-y) dy - \sum_{\gamma=0}^{N} \sum_{\alpha=0}^{m-2} (-1)^\alpha C^{(L)}_{\gamma,\alpha} G_m^{(\alpha)}(x-h\gamma) - \\ &\quad -(-1)^{m-1} \sum_{\gamma=0}^{N} C^{(W)}_{\gamma,m-1} G_m^{(m-1)}(x-h\gamma) \Bigg) dx.\end{aligned}$$

From last expression after some simplification we have

$$\begin{aligned}
\|\ell\|^2_{W_2^{(m,m-1)*}} = (-1)^m \Bigg[\int_0^1\int_0^1 p(x)p(y)G_m(x-y)dxdy - \\
-2\sum_{\alpha=0}^{m-2}(-1)^\alpha\sum_{\gamma=0}^{N}C^{(L)}_{\gamma,\alpha}\int_0^1 p(x)G_m^{(\alpha)}(x-h\gamma)dx+ \\
+\sum_{\alpha_1=0}^{m-2}\sum_{\alpha_2=0}^{m-2}(-1)^{\alpha_2}\sum_{\gamma=0}^{N}\sum_{\beta=0}^{N}C^{(L)}_{\gamma,\alpha_1}C^{(L)}_{\beta,\alpha_2}G_m^{(\alpha_1+\alpha_2)}(h\beta-h\gamma)- \\
-2\sum_{\beta=0}^{N}C^{(W)}_{\beta,m-1}\Bigg((-1)^{m-1}\int_0^1 p(x)G_m^{(m-1)}(x-h\beta)dx - \\
-\sum_{\alpha=0}^{m-2}(-1)^\alpha\sum_{\gamma=0}^{N}C^{(L)}_{\gamma,\alpha}G_m^{(\alpha+m-1)}(h\beta-h\gamma)\Bigg)+ \\
+(-1)^{m-1}\sum_{\beta=0}^{N}\sum_{\gamma=0}^{N}C^{(W)}_{\beta,m-1}C^{(W)}_{\gamma,m-1}G_m^{(2m-2)}(h\beta-h\gamma)\Bigg].
\end{aligned} \tag{16}$$

It can be seen from the equality (11) that, the square of the error functional norm is a multivariate function concerning coefficients $C^{(W)}_{\beta,m-1}$. Given the condition (13), we consider the Lagrange function to find the conditional minimum of the expression (16)

$$\Phi(\mathbf{C},d) = \|\ell\|^2_{W_2^{(m,m-1)*}} - 2(-1)^m d(\ell, e^{-x}),$$

here $\mathbf{C} = (C^{(W)}_{0,m-1}, C^{(W)}_{1,m-1}, \dots, C^{(W)}_{N,m-1})$, and d is unknown real number. Also, we have

$$(\ell, e^{-x}) = \int_0^1 p(x)e^{-x}dx - \sum_{\gamma=0}^{N}\sum_{\alpha=0}^{m-2}(-1)^\alpha C^{(L)}_{\gamma,\alpha}e^{-h\beta} - (-1)^{m-1}\sum_{\gamma=0}^{N}C^{(W)}_{\gamma,m-1}e^{-h\beta} = 0.$$

In that case, equating to 0 the partial derivatives of the function Φ by $\mathbf{C}$ and d, we get the following system of linear equations

$$\sum_{\gamma=0}^{N}C^{(W)}_{\gamma,m-1}G_m^{(2m-2)}(h\beta-h\gamma) + de^{-h\beta} = F_m(h\beta), \quad \beta=0,1,\dots,N, \tag{17}$$

$$\sum_{\gamma=0}^{N}C^{(W)}_{\gamma,m-1}e^{-h\gamma} = t_m, \tag{18}$$

here,

$$F_m(h\beta) = \int_0^1 p(x)G_m^{(m-1)}(x-h\beta)dx - \sum_{\alpha=0}^{m-2}\sum_{\gamma=0}^{N}C^{(L)}_{\gamma,\alpha}G_m^{(\alpha+m-1)}(h\gamma-h\beta),$$

$$t_m = (-1)^{m-1}\left(\int_0^1 p(x)e^{-x}dx - \sum_{\gamma=0}^{N}\sum_{\alpha=0}^{m-2}(-1)^\alpha C^{(L)}_{\gamma,\alpha}e^{-h\beta}\right).$$

A quadrature formula with coefficients $\mathring{C}^{(W)}_{\beta,m-1}$ ($\beta = \overline{0,N}$ corresponding to this mini - mum is called *optimal*, and $\mathring{C}^{(W)}_{\beta,m-1}$ ($\beta = \overline{0,N}$ are called *optimal coefficients* of the quadrature formula.

5 Conclusion

This work discussed the problem of constructing an optimal quadrature formula with high accuracy for the approximate calculation of the weighted integrals (7). We analyzed the error of the quadrature formula in a specific form and studied the problem of determining the analytical form of the coefficients of the quadrature formula that minimizes the norm of its error functional. Subsequently, we derived the system of linear equations for the coefficients of optimal quadrature formulas over the interval $[0, 1]$.

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ВЕСОВАЯ ОПТИМАЛЬНАЯ КВАДРАТУРНАЯ ФОРМУЛА С ПРОИЗВОДНЫМИ В ГИЛЬБЕРТОВОМ ПРОСТРАНСТВЕ

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В настоящей статье обсуждается задача построения оптимальной квадратурной формулы в смысле Сарда для численного интегрирования весовых интегралов в гильбертовом пространстве вещественных функций. Первоначально находится норма функционала погрешности с помощью экстремальной функции функционала погрешности квадратурной формулы. Поскольку функционал погрешности определен на гильбертовом пространстве, то построенная нами квадратурная формула точна для нулей этого пространства, то есть выполняются условия, что влияние функционала погрешности на эти функции равно нулю. Затем строится функция Лагранжа для нахождения условного экстремума нормы функционала погрешности. Тем самым получается система линейных уравнений для коэффициентов оптимальной квадратурной формулы.

Ключевые слова: квадратурная формула с производными, экстремальная функция, функционал погрешности, оптимальный коэффициент, функция Лагранжа.

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