

Optimal Difference Formulas for the Approximate Solution of the Second-Order Cauchy Problem

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Abstract. It is well established that the Cauchy problem for second-order differential equations serves as a canonical model of gradient conservative or weakly damped dynamical systems, widely applied in mechanics, astronomy, molecular and structural dynamics, acoustics, and radio-frequency systems. Exact solutions are usually attainable only for linear or simple functions, whereas in most other cases approximate solution methods are employed. In this work, we make use of the Sobolev method to develop an optimal explicit difference formula of the Störmer type for the Cauchy problem of second-order differential equations.

1. INTRODUCTION

Ordinary differential equations are widely used in various fields of science, engineering, and mathematics for modeling physical, biological, and dynamical systems [1–5].

The analytical solution of ordinary differential equations presents significant difficulties or becomes impossible for complex differential equations [6–8]. Therefore, numerical methods play an important role in approximating the solutions of such equations.

Among the types of problems for ordinary differential equations, the Cauchy problem is of particular importance, where the values of the unknown function and its derivatives are specified at the initial point. Many researchers have developed various methods for the approximate solution of ordinary differential equations with initial conditions. In [9], spectral schemes were developed

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using Legendre polynomials as basis functions. Moreover, spectral methods are based on representing the solution as a series of basis functions, such as Legendre polynomials, Chebyshev polynomials, and Fourier series ([6], [10], [11]).

In [12], the Euler method and the fourth-order Runge–Kutta method are applied to the numerical solution of the Cauchy problem.

In [13], efficient multi-step block methods for the direct solution of general second-order Cauchy problems are considered. This work is an extension of [14].

It should be noted that the literature contains a wide variety of methods for the direct approximation of the solution to the Cauchy problem [15–18]. It is known that the first appearance of block methods is associated with [19]. A considerable number of works have been published on this topic. An interesting monograph in this field was written by Brugnano and Trigiante [20].

In [21], an implicit three-point block method is proposed for the direct solution of second-order ordinary differential equations.

In [22], new types of functionally fitted block methods are proposed for second-order Cauchy problems.

In [23], a transformation of an integro-differential equation into a system of weakly coupled local evolution equations is presented.

In [24], an implicit optimal difference formula in the Sobolev space $L_2^{(3)}(0, 1)$ was constructed for the approximate solution of the Cauchy problem for a second-order differential equation, and an error bound for the constructed formula was derived.

For the approximate solution of first-order Cauchy problems, optimal difference formulas in Hilbert spaces were constructed using the Sobolev method in [25–29]. By using this method, it is possible to construct not only optimal difference formulas but also optimal quadrature and interpolation formulas (for example, [30–32]).

In this work, we consider the approximate solution of the following second-order ordinary differential equation

$$y'' = f(x, y), \quad x \in [0, 1], \quad (1.1)$$

subject to the initial conditions

$$y(0) = y_0, \quad y'(0) = u_0. \quad (1.2)$$

Let the differential equation in the form (1.1) with the initial conditions (1.2) have a unique solution on the segment $x \in [0, 1]$. It is required to find the approximate solution of this problem on the interval $[0, 1]$. Let us divide this interval into N parts of length $h = \frac{1}{N}$, and denote the solution of problem (1.1)–(1.2) at the points $x_n = nh$, $n = 0, 1, \dots, N$ by $y(x_n)$, while its approximate values will be denoted by $\tilde{y}_n$.

2. PROBLEM STATEMENT

To obtain an approximate solution of problem (1.1)–(1.2), we consider the following general difference formula [33, 34]:

$$\sum_{\beta=0}^k C[\beta] \varphi[\beta] - h^2 \sum_{\beta=0}^k C^{(\text{II})}[\beta] \varphi''[\beta] \cong 0. \quad (2.1)$$

Here, $C[\beta]$ and $C^{(\text{II})}[\beta]$ are the unknown coefficients of the difference formula, $h = \frac{1}{N}$, $[\beta] = h\beta$, ($\beta = 0, 1, \dots, k$), and $\varphi(x) \in L_2^{(4)}(0, 1)$. $L_2^{(4)}(0, 1)$ is a Sobolev space, which is defined as follows:

$$L_2^{(4)}(0, 1) = \left\{ \varphi : [0, 1] \rightarrow \mathbb{R} \mid \varphi^{(3)}(x) \text{ is absolutely continuous on } [0, 1], \varphi^{(4)}(x) \in L_2(0, 1) \right\}.$$

In the space $L_2^{(4)}(0, 1)$, the inner product of any two functions φ and ψ is defined as follows [35]:

$$\langle \psi, \varphi \rangle = \int_0^1 \varphi^{(4)}(x) \psi^{(4)}(x) dx. \quad (2.2)$$

Similarly, in the space $L_2^{(4)}(0, 1)$, the norm of a function corresponding to the inner product (2.2) is defined as follows:

$$\|\varphi\|_{L_2^{(4)}(0, 1)} = \left(\int_0^1 (\varphi^{(4)}(x))^2 dx \right)^{\frac{1}{2}} \quad (2.3)$$

In the considered formula (2.1), the difference between the given sums

$$\begin{aligned} (\ell, \varphi) &= \sum_{\beta=0}^k C[\beta] \varphi[\beta] - h^2 \sum_{\beta=0}^k C^{(\text{II})}[\beta] \varphi''[\beta] \\ &= \int_{-\infty}^{\infty} \left[\sum_{\beta=0}^k C[\beta] \delta(x - h\beta) - h^2 \sum_{\beta=0}^k C^{(\text{II})}[\beta] \delta''(x - h\beta) \right] \varphi(x) dx \end{aligned} \quad (2.4)$$

is called the error of the difference formula (2.1). For the obtained expression (2.4), the following error functional belonging to the dual space $L_2^{(4)*}(0, 1)$ corresponds, and it has the form

$$\ell(x) = \sum_{\beta=0}^k C[\beta] \delta(x - h\beta) - h^2 \sum_{\beta=0}^k C^{(\text{II})}[\beta] \delta''(x - h\beta), \quad (2.5)$$

where $L_2^{(4)*}(0, 1)$ is the dual space of $L_2^{(4)}(0, 1)$, and $\delta(x)$ is the Dirac delta function. Based on the Cauchy–Schwarz inequality, we obtain the following estimate:

$$|(\ell, \varphi)| \leq \|\ell\|_{L_2^{(4)*}} \cdot \|\varphi\|_{L_2^{(4)}}. \quad (2.6)$$

Thus, the error (2.4) of the difference formula (2.1) is bounded from above by the norm of the error functional (2.5) taken from the dual space $L_2^{(4)*}(0, 1)$ and the norm of the functions φ taken from the space $L_2^{(4)}(0, 1)$. For the error functional ℓ , the following conditions hold:

$$(\ell, x^\alpha) = 0, \quad \alpha = 0, 1, 2, 3. \quad (2.7)$$

From the condition (2.7) above, we obtain the following orthogonality conditions for the coefficients:

$$\sum_{\beta=0}^k C[\beta] = 0, \quad (2.8)$$

$$\sum_{\beta=0}^k C[\beta] \cdot (h\beta) = 0, \quad (2.9)$$

$$\sum_{\beta=0}^k C[\beta] \cdot (h\beta)^2 - 2h^2 \sum_{\beta=0}^k C^{(II)}[\beta] = 0, \quad (2.10)$$

$$\sum_{\beta=0}^k C[\beta] \cdot (h\beta)^3 - 6h^2 \sum_{\beta=0}^k C^{(II)}[\beta] (h\beta) = 0. \quad (2.11)$$

Thus, the norm of the error functional depends on the coefficients $C[\beta]$ va $C^{(II)}[\beta]$, as well as on the grid points $h\beta$ ($\beta = 0, 1, \dots, N$). In the optimal difference formula under consideration, the norm of the error functional is minimized with respect to the coefficients $C^{(II)}[\beta]$. The coefficients $C[\beta]$ are chosen, in the sense of Dahlquist, to be stable so that they satisfy condition (2.8). The norm of the functional is a number. From this, the following problems arise.

Problem 2.1. *To find the expression of the square of the norm of the error functional of the difference formula (2.1) in the space $L_2^{(4)*}(0, 1)$.*

It is clear that the norm of the error functional ℓ depends on the coefficients $C^{(II)}[\beta]$ and the nodes $[\beta]$. The problem of minimization of the quantity $\|\ell\|$ by coefficients $C^{(II)}[\beta]$ is a linear problem and by nodes $[\beta]$ is, in general, a complicated and non-linear problem. We consider the problem of minimization of the quantity $\|\ell\|$ by coefficients $C^{(II)}[\beta]$ when the nodes $[\beta]$ are fixed.

If there are coefficients $\overset{\circ}{C}^{(II)}[\beta]$ that minimize the norm of the error functional, that is,

$$\left\| \overset{\circ}{\ell} \right\|_{L_2^{(4)*}(0, 1)} = \inf_{C^{(II)}[\beta]} \left\| \ell \right\|_{L_2^{(4)*}(0, 1)} \quad (2.12)$$

then they are called the *optimal coefficients* and the corresponding difference formula

$$\sum_{\beta=0}^k C[\beta] \varphi[\beta] - h^2 \sum_{\beta=0}^k \overset{\circ}{C}^{(II)}[\beta] \varphi''[\beta] \cong 0$$

is called the *optimal difference formula* in the space $L_2^{(4)}(0, 1)$.

Thus, in order to construct the optimal difference formula in the space $L_2^{(4)}(0, 1)$ we need to solve the next problem.

Problem 2.2. *Find the coefficients $\overset{\circ}{C}^{(II)}[\beta]$ that give the quantity (2.12) when the nodes $[\beta]$ are fixed.*

3. THE UPPER BOUND OF THE ERROR OF THE DIFFERENCE FORMULA

To calculate the norm of the error functional ℓ , we use the concept of the extremal function introduced by Sergey Sobolev [35], that is,

$$|(\ell, \psi_\ell)| = \|\ell\|_{L_2^{(4)*}(0,1)} \cdot \|\psi_\ell\|_{L_2^{(4)}(0,1)},$$

where ψ_ℓ is the extremal function.

Since the space $L_2^{(4)}(0,1)$ is a Hilbert space, by the Riesz theorem on the general form of a linear continuous functional (see [36]), there exists a unique function ψ_ℓ in this space that satisfies the following equalities:

$$(\ell, \varphi) = \langle \psi_\ell, \varphi \rangle_{L_2^{(4)}(0,1)},$$

and

$$\|\ell\| = \|\psi_\ell\|,$$

where $\langle \psi_\ell, \varphi \rangle_{L_2^{(4)}(0,1)}$ denotes the inner product of the functions ψ_ℓ and φ in the space $L_2^{(4)}(0,1)$

For the extremal function of the error functional ℓ and for the square of its norm, the following theorems hold:

Theorem 3.1. *In the Sobolev space $L_2^{(4)}(0,1)$, for the extremal function of the error functional ℓ of the difference formula (2.1), the following expression holds:*

$$\psi_\ell(x) = \ell(x) * G_4(x) + P_3(x),$$

where $G_4(x) = \frac{|x|^7}{2 \cdot 7!}$ and it satisfies the equality $\frac{d^8 G_4(x)}{dx^8} = \delta(x)$, and $P_3(x)$ is a cubic polynomial.

Theorem 3.2. *For the square of the norm of the error functional corresponding to the difference formula (2.1), the following equality holds:*

$$\begin{aligned} \|\ell\|_{L_2^{(4)*}(0,1)}^2 &= \sum_{\beta=0}^k \sum_{\gamma=0}^k C[\beta] C[\gamma] G_3(h\beta - h\gamma) \\ &\quad - 2h^2 \sum_{\beta=0}^k \sum_{\gamma=0}^k C[\beta] C^{(\text{II})}[\gamma] G_4''(h\beta - h\gamma) + h^4 \sum_{\beta=0}^k \sum_{\gamma=0}^k C^{(\text{II})}[\beta] C^{(\text{II})}[\gamma] G_4^{IV}(h\beta - h\gamma). \end{aligned}$$

Here $G_4(h\beta - h\gamma) = \frac{|h\beta - h\gamma|^7}{2 \cdot 7!}$, $G_4''(h\beta - h\gamma) = \frac{|h\beta - h\gamma|^5}{2 \cdot 5!}$, $G_4^{IV}(h\beta - h\gamma) = \frac{|h\beta - h\gamma|^3}{2 \cdot 3!}$.

The proof of this theorem follows from the proofs of Theorems 3.1 and 3.2 in [37] for the case $m = 4$.

Thus, **Problem 2.1** is solved.

4. FINDING THE CONDITIONAL MINIMUM FOR THE NORM OF THE ERROR FUNCTIONAL

Now we proceed to solve **Problem 2.2**. For this, we minimize the square of the norm of the error functional ℓ of the difference formula (2.1) with respect to the coefficients $C^{(\text{II})}[\beta]$. That is, we use the method of Lagrange multipliers, which is applied in finding the extremum of a multivariable function.

Thus, we construct the following Lagrangian function:

$$\Lambda(C^{(II)}, d) = \|\ell\|^2 - 2 \sum_{\alpha=0}^3 d_{\alpha}(\ell, x^{\alpha}).$$

From the function $\Lambda(C^{(II)}, d)$, we set the partial derivatives with respect to $C^{(II)}[\beta]$ and d_{α} equal to zero:

$$\begin{aligned} \frac{\partial \Lambda}{\partial C^{(II)}[\beta]} &= 0, \quad \beta = 0, 1, \dots, k, \\ \frac{\partial \Lambda}{\partial d_{\alpha}} &= 0, \quad \alpha = 0, 1, 2, 3. \end{aligned}$$

As a result, we obtain the following system of equations:

$$h^2 \sum_{\gamma=0}^k \overset{\circ}{C}^{(II)}[\gamma] G_4^{(IV)}(h\beta - h\gamma) + d_0 + d_1 \cdot [\beta] = \sum_{\gamma=0}^k C[\gamma] G_4''(h\beta - h\gamma), \quad \beta = 0, 1, \dots, k, \quad (4.1)$$

$$\sum_{\gamma=0}^k \overset{\circ}{C}^{(II)}[\gamma] = 1, \quad (4.2)$$

$$\sum_{\gamma=0}^k \overset{\circ}{C}^{(II)}[\gamma] \cdot \gamma = k - 1. \quad (4.3)$$

The solution of the system of linear equations (4.1)–(4.3) with respect to the unknowns $\overset{\circ}{C}^{(II)}[\beta]$, d_0 , and d_1 represents the critical points of the function $\Lambda(C^{(II)}, d)$. The solutions obtained, in accordance with conditions (2.8)–(2.11), provide the conditional minimum of the norm of the error functional. It is known that, in the sense of Dahlquist [38, 39], the stability of the difference formula (2.1) depends only on the coefficients $C[\beta]$, $\beta = 0, 1, \dots, k$. Thus, in this work we choose the coefficients $C[\beta]$ so that they are stable in the sense of Dahlquist and satisfy the equality $\sum_{\gamma=0}^k C[\gamma] = 0$, as follows:

$$C[\gamma] = \begin{cases} 0, & \text{for } \gamma = 0, \dots, k-3, \\ 1, & \text{for } \gamma = k-2, \\ -2, & \text{for } \gamma = k-1, \\ 1, & \text{for } \gamma = k. \end{cases} \quad (4.4)$$

In the system of equations (4.1)–(4.3), we set $\overset{\circ}{C}^{(II)}[k] = 0$ and consider constructing an explicit (Störmer type) difference formula. In that case, the system (4.1)–(4.3) takes the following form:

$$h^2 \sum_{\gamma=0}^{k-1} \overset{\circ}{C}^{(II)}[\gamma] G_4^{(IV)}(h\beta - h\gamma) + d_0 + d_1 \cdot [\beta] = \sum_{\gamma=0}^k C[\gamma] G_4''(h\beta - h\gamma), \quad \beta = 0, 1, \dots, k-1, \quad (4.5)$$

$$\sum_{\gamma=0}^{k-1} \overset{\circ}{C}^{(II)}[\gamma] = 1, \quad (4.6)$$

$$\sum_{\gamma=0}^{k-1} \overset{\circ}{C}^{(II)}[\gamma] \cdot \gamma = k-1, \quad (4.7)$$

where $\overset{\circ}{C}^{(II)}[\gamma]$, $\gamma = \overline{0, k-1}$, are the unknown coefficients, and d_0, d_1 are unknown constants.

Now, by solving the system of equations (4.5)–(4.7) using Sobolev's method, we obtain the optimal explicit coefficients.

5. FINDING THE COEFFICIENTS OF THE OPTIMAL EXPLICIT DIFFERENCE FORMULA

Theorem 5.1. *In the Sobolev space $L_2^{(4)}(0, 1)$, the coefficients of the unique explicit optimal difference formula of Störmer type corresponding to the difference formula (2.1) are determined as follows:*

$$\begin{aligned} \overset{\circ}{C}^{(II)}[0] &= \frac{3(1+q)q^{k-1}}{10(1-q^{2k-2})(1-q)}, \\ \overset{\circ}{C}^{(II)}[\beta] &= -\frac{3q^{k-1}}{10(1-q^{2k-2})}(q^\beta - q^{-\beta}), \quad \beta = \overline{1, k-3}, \\ \overset{\circ}{C}^{(II)}[k-2] &= \frac{1}{20} + \frac{3(q - q^{2k-3})}{10(1-q^{2k-2})}, \\ \overset{\circ}{C}^{(II)}[k-1] &= \frac{19}{20} - \frac{3(q + q^{2k-2})}{10(1-q)(1-q^{2k-2})}. \end{aligned}$$

Here, $q = \sqrt{3} - 2$ is the root of the quadratic Euler polynomial.

Proof. We denote the right-hand side of equation (4.5) by $f_4(h\beta)$:

$$f_4[\beta] = \sum_{\gamma=0}^k C[\gamma] G_4''(h\beta - h\gamma), \quad \beta = \overline{0, k-1}. \quad (5.1)$$

Now, we find the explicit form of expression (5.1) in the form of a piecewise function.

Using $G_4''(h\beta - h\gamma) = \frac{|h\beta - h\gamma|^5}{2 \cdot 5!}$ and expression (4.4), we can rewrite equality (5.1) in the following form:

$$f_4[\beta] = \sum_{\gamma=0}^k C[\gamma] \frac{|h\beta - h\gamma|^5}{2 \cdot 5!} = \frac{h^5}{2 \cdot 5!} \left[|\beta - k + 2|^5 - 2|\beta - k + 1|^5 + |\beta - k|^5 \right]. \quad (5.2)$$

In (5.2), we expand the absolute value for $\beta \in \overline{0, k-2}$:

$$\begin{aligned} f_4[\beta] &= -\frac{h^5}{2 \cdot 5!} \left[(\beta - k + 2)^5 - 2(\beta - k + 1)^5 + (\beta - k)^5 \right] \\ &= -\frac{h^5}{4!} \left[2\beta^3 - 6\beta^2(k-1) + \beta(6(k-1)^2 + 1) - (k-1)(2(k-1)^2 + 1) \right]. \end{aligned}$$

For $\beta = k-1$ we obtain:

$$f_4[\beta] = \frac{h^5}{2 \cdot 5!} \left[|k-1-k+2|^5 - 2|k-1-k+1|^5 + |k-1-k|^5 \right] = \frac{h^5}{2 \cdot 5!} \cdot 2 = \frac{h^5}{5!}.$$

Thus,

$$f_4[\beta] = \begin{cases} -\frac{h^5}{4!} \left[2\beta^3 - 6\beta^2(k-1) + \beta(6(k-1)^2 + 1) - (k-1)(2(k-1)^2 + 1) \right], & \beta = \overline{0, k-2}, \\ \frac{h^5}{5!}, & \beta = k-1. \end{cases} \quad (5.3)$$

Now we can write equation (4.5) in the following form:

$$h^2 \sum_{\gamma=0}^{k-1} \overset{\circ}{C}^{(\text{II})}[\gamma] G_4^{IV}(h\beta - h\gamma) + d_0 + d_1 \cdot [\beta] = f_4[\beta]. \quad (5.4)$$

Denoting the right-hand side of equation (5.4) by $U_4[\beta]$, we can also write it in the following form:

$$U_4[\beta] = V_4[\beta] + d_0 + d_1 \cdot [\beta]. \quad (5.5)$$

In equation (5.5), $V_4[\beta]$ is given by

$$V_4[\beta] = h^2 \sum_{\gamma=0}^{k-1} \overset{\circ}{C}^{(\text{II})}[\gamma] G_4^{IV}(h\beta - h\gamma). \quad (5.6)$$

Since in equation (5.6) we have $G_4^{IV}(h\beta - h\gamma) = \frac{|h\beta - h\gamma|^3}{2 \cdot 3!}$, it follows that

$$V_4[\beta] = h^2 \sum_{\gamma=0}^{k-1} \overset{\circ}{C}^{(\text{II})}[\gamma] \frac{|h\beta - h\gamma|^3}{2 \cdot 3!} = \frac{h^5}{2 \cdot 3!} \sum_{\gamma=0}^{k-1} \overset{\circ}{C}^{(\text{II})}[\gamma] |\beta - \gamma|^3.$$

For $\beta < 0$ we have

$$V_4[\beta] = -\frac{h^5}{2 \cdot 3!} \sum_{\gamma=0}^{k-1} \overset{\circ}{C}^{(\text{II})}[\gamma] (\beta - \gamma)^3 = -\frac{h^5}{2 \cdot 3!} \left[\beta^3 - 3\beta^2(k-1) + 3\beta \sum_{\gamma=0}^{k-1} \overset{\circ}{C}^{(\text{II})}[\gamma] \cdot \gamma^2 - \sum_{\gamma=0}^{k-1} \overset{\circ}{C}^{(\text{II})}[\gamma] \cdot \gamma^3 \right],$$

and for $\beta > k-1$ we have

$$V_4[\beta] = \frac{h^5}{2 \cdot 3!} \left[\beta^3 - 3\beta^2(k-1) + 3\beta \sum_{\gamma=0}^{k-1} \overset{\circ}{C}^{(\text{II})}[\gamma] \cdot \gamma^2 - \sum_{\gamma=0}^{k-1} \overset{\circ}{C}^{(\text{II})}[\gamma] \cdot \gamma^3 \right].$$

We can rewrite $U_4[\beta]$ as follows:

$$U_4[\beta] = \begin{cases} -\frac{h^5}{2 \cdot 3!} \left[\beta^3 - 3\beta^2(k-1) + d_0^- + d_1^-[\beta] \right], & \beta < 0, \\ f_4[\beta], & \beta = 0, 1, \dots, k-1, \\ \frac{h^5}{2 \cdot 3!} \left[\beta^3 - 3\beta^2(k-1) + d_0^+ + d_1^+[\beta] \right], & \beta > k-1, \end{cases} \quad (5.7)$$

Here $d_0^- = d_0 + \frac{h^5}{2 \cdot 3!} \sum_{\gamma=0}^{k-1} \overset{\circ}{C}^{(\text{II})}[\gamma] \cdot \gamma^3$, $d_1^- = d_1 - \frac{h^4}{4} \sum_{\gamma=0}^{k-1} \overset{\circ}{C}^{(\text{II})}[\gamma] \cdot \gamma^2$, $d_0^+ = d_0 - \frac{h^5}{2 \cdot 3!} \sum_{\gamma=0}^{k-1} \overset{\circ}{C}^{(\text{II})}[\gamma] \cdot \gamma^3$,

$$d_1^+ = d_1 + \frac{h^4}{4} \sum_{\gamma=0}^{k-1} \overset{\circ}{C}^{(\text{II})}[\gamma] \cdot \gamma^2.$$

Now, substituting $\beta = 0$ and $\beta = k - 1$ into equation (5.7), we obtain the following results.

For $\beta = 0$ we have

$$d_0^- = \frac{h^5}{4!}(k-1)(2(k-1)^2 + 1). \quad (5.8)$$

For $\beta = k - 1$ we obtain

$$d_0^+ = \frac{h^5}{5!} + \frac{h^5}{3!}(k-1)^3 - d_1^+ h(k-1). \quad (5.9)$$

Equations (5.8) and (5.9) thus give the explicit forms of d_0^- and d_0^+ corresponding to the boundary values $\beta = 0$ and $\beta = k - 1$.

Substituting expressions (5.8) and (5.9) into equation (5.7), we obtain the final form of $U_4[\beta]$ as follows:

$$U_4[\beta] = \begin{cases} -\frac{h^5}{4!} \left[2\beta^3 - 6\beta^2(k-1) + (k-1)(2(k-1)^2 + 1) \right] + d_1^- [\beta], & \beta < 0, \\ f_4[\beta], & \beta = 0, 1, \dots, k-1, \\ \frac{h^5}{4!} \left[2\beta^3 - 6\beta^2(k-1) + 4(k-1)^3 + \frac{1}{5} \right] + d_1^+ h(\beta - k + 1), & \beta > k-1. \end{cases} \quad (5.10)$$

Since $\overset{\circ}{C}^{(II)}[\gamma] = 0$ for $\beta < 0$ and $\beta > k - 1$, we can rewrite $U_4[\beta]$ in the convolution form as

$$U_4[\beta] = h^2 \overset{\circ}{C}^{(II)}[\beta] * G_4^{IV}[\beta] + d_0 + d_1 \cdot [\beta]. \quad (5.11)$$

Now, from equation (5.11), in order to determine the coefficients $\overset{\circ}{C}^{(II)}[\beta]$, we make use of the following operator [40]:

$$D_2[\beta] = \frac{6}{h^4} \begin{cases} A_2 q^{|\beta|-1}, & |\beta| \geq 2, \\ 1 + A_2, & |\beta| = 1, \\ -8 + \frac{A_2}{q}, & \beta = 0. \end{cases} \quad (5.12)$$

where $A_2 = 6\sqrt{3}q$ and $q = \sqrt{3} - 2$.

Applying the operator $D_2[\beta]$ to both sides of equation (5.11), we obtain

$$U_4[\beta] * D_2[\beta] = h^2 \overset{\circ}{C}^{(II)}[\beta] * G_4^{IV}[\beta] * D_2[\beta] + d_0 * D_2[\beta] + d_1 \cdot [\beta] * D_2[\beta].$$

Since $G_4^{IV}[\beta] * D_2[\beta] = \delta[\beta]$, $\delta[\beta] * \overset{\circ}{C}^{(II)}[\beta] = \overset{\circ}{C}^{(II)}[\beta]$, $D_2[\beta] * d_0 = 0$, and $D_2[\beta] * d_1 \cdot [\beta] = 0$, we can write

$$\overset{\circ}{C}^{(II)}[\beta] = h^{-1} D_2[\beta] * U_4[\beta]. \quad (5.13)$$

Expanding equation (5.13), we obtain

$$\overset{\circ}{C}^{(II)}[\beta] = h^{-1} \left\{ \frac{h^5}{5!} [\beta - k + 1] + \sum_{\gamma=1}^{\infty} D_2[\beta + \gamma] (U_4^-[-\gamma] - f[-\gamma]) + \sum_{\gamma=k}^{\infty} D_2[\beta - \gamma] (U_4^+[\gamma] - f[\gamma]) \right\}, \quad (5.14)$$

here, $U_4^-[\gamma]$ and $U_4^+[\gamma]$ are the expressions of equation (5.10) for $\beta < 0$ and $\beta > k-1$, respectively, while $f[\gamma]$ denotes the expression of $f_4[\gamma]$ for $\beta = \overline{0, k-2}$.

Now, by applying operator (5.12) to formula (5.14), we separately determine the form of the optimal coefficients $\mathring{C}^{(II)}[\beta]$ for $\beta = \overline{1, k-3}$ and $\beta = k-2$:

$$\mathring{C}^{(II)}[\beta] = aq^\beta + bq^{k-1-\beta}, \quad \beta = \overline{1, k-3}, \quad (5.15)$$

$$\mathring{C}^{(II)}[k-2] = \frac{1}{20} + aq^{k-2} + bq,$$

where a and b are respectively equal to the following:

$$a = \frac{6}{h^5} A_2 \sum_{\gamma=1}^{\infty} q^{\gamma-1} (U_4^-[-\gamma] - f[-\gamma]), \quad (5.16)$$

$$b = \frac{A_2}{20q} + \frac{6}{h^5} A_2 \sum_{\gamma=1}^{\infty} q^{\gamma-1} (U_4^+[\gamma+k-1] - f[\gamma+k-1]) \quad (5.17)$$

If we determine the coefficients $\mathring{C}^{(II)}[0]$ and $\mathring{C}^{(II)}[k-1]$ using equations (4.6) and (4.7), respectively, we obtain the following:

$$\begin{aligned} \mathring{C}^{(II)}[0] &= -\frac{1}{20(k-1)} - \frac{(a-b)(1-q^{k-1})}{6(k-1)} - \frac{aq - bq^{k-1}}{1-q}, \\ \mathring{C}^{(II)}[k-1] &= \frac{19k-18}{20(k-1)} + \frac{(a-b)(1-q^{k-1})}{6(k-1)} + \frac{aq^{k-1} - bq}{1-q}. \end{aligned}$$

Now, by expanding both the left-hand side and the right-hand side of equation (4.5) in powers of β and equating the corresponding coefficients, we determine the values of a and b . In our case, the right-hand side of equation (4.3) has been evaluated in formula (5.3). Therefore, we can rewrite the right-hand side as

$$S + d_0 + d_1 \cdot [\beta],$$

where

$$S = h^2 \sum_{\gamma=0}^{k-1} \mathring{C}^{(II)}[\gamma] G_4^{IV}(h\beta - h\gamma). \quad (5.18)$$

Since in the sum (5.18) we have

$$G_4^{IV}(h\beta - h\gamma) = \frac{|h\beta - h\gamma|^3}{12},$$

we can rewrite and compute it as follows:

$$\begin{aligned} S &= h^2 \sum_{\gamma=0}^{\beta} \mathring{C}^{(II)}[\gamma] \frac{(h\beta - h\gamma)^3}{12} - h^2 \sum_{\gamma=\beta}^{k-1} \mathring{C}^{(II)}[\gamma] \frac{(h\beta - h\gamma)^3}{12} \\ &= h^2 \sum_{\gamma=0}^{\beta} \mathring{C}^{(II)}[\gamma] \frac{(h\beta - h\gamma)^3}{6} - h^2 \sum_{\gamma=0}^{k-1} \mathring{C}^{(II)}[\gamma] \frac{(h\beta - h\gamma)^3}{12} = K_1 - K_2. \end{aligned}$$

First, we calculate the sum K_2 :

$$K_2 = h^2 \sum_{\gamma=0}^{k-1} \overset{\circ}{C}^{(\text{II})}[\gamma] \frac{(h\beta - h\gamma)^3}{12} = \frac{h^5}{12} \beta^3 - \frac{h^5(k-1)}{4} \beta^2 + \frac{h^3}{4} \beta \sum_{\gamma=0}^{k-1} \overset{\circ}{C}^{(\text{II})}[\gamma] [\gamma]^2 - \frac{h^2}{12} \sum_{\gamma=0}^{k-1} \overset{\circ}{C}^{(\text{II})}[\gamma] [\gamma]^3.$$

Now we simplify the sum K_1 :

$$K_1 = h^2 \sum_{\gamma=0}^{\beta} \overset{\circ}{C}^{(\text{II})}[\gamma] \frac{(h\beta - h\gamma)^3}{6} = \frac{h^2}{6} \overset{\circ}{C}^{(\text{II})}[0] (h\beta)^3 + h^2 \sum_{\gamma=1}^{\beta} \overset{\circ}{C}^{(\text{II})}[\gamma] \frac{(h\beta - h\gamma)^3}{6}.$$

Substituting the coefficients $\overset{\circ}{C}^{(\text{II})}[\gamma]$ from formula (5.15), we obtain

$$K_1 = \frac{h^2}{6} \overset{\circ}{C}^{(\text{II})}[0] (h\beta)^3 + \frac{h^5}{6} \sum_{\gamma=1}^{\beta} (h\beta - h\gamma)^3 (aq^{\gamma} + bq^{k-1-\gamma}). \quad (5.19)$$

In formula (5.19), let us change variables: set $\beta - \gamma = \gamma_1$ and denote γ_1 again by γ . Then the summation limit changes to $\beta - 1$, and we have

$$K_1 = \frac{h^2}{6} \overset{\circ}{C}^{(\text{II})}[0] (h\beta)^3 + \frac{h^5}{6} \left[a \sum_{\gamma=0}^{\beta-1} q^{\beta-\gamma} \gamma^3 + b \sum_{\gamma=0}^{\beta-1} q^{k-1-\beta+\gamma} \gamma^3 \right]. \quad (5.20)$$

We compute this sum using the following known formula:

$$\sum_{\gamma=0}^{n-1} q^{\gamma} \gamma^p = \frac{1}{1-q} \sum_{i=0}^p \left(\frac{q}{1-q} \right)^i \Delta^i 0^p - \frac{q^n}{1-q} \sum_{i=0}^p \left(\frac{q}{1-q} \right)^i \Delta^i \gamma^p \Big|_{\gamma=n}, \quad (5.21)$$

where $\Delta^i \gamma^p$ denotes the i -th order finite difference of γ^p , and

$$\Delta^i 0^p = \Delta^i \gamma^p \Big|_{\gamma=0}, \quad \Delta^i \gamma^p = \sum_{\mu=0}^k \binom{k}{\mu} \gamma^{p-\mu} \Delta^i 0^{\mu}.$$

If in formula (5.21) we substitute q^{-1} in place of q , we obtain the following summation formula:

$$\sum_{\gamma=0}^{n-1} q^{-\gamma} \gamma^p = \frac{q}{q-1} \sum_{i=0}^p \left(\frac{1}{q-1} \right)^i \Delta^i 0^p - \frac{q^{-n+1}}{q-1} \sum_{i=0}^p \left(\frac{1}{1-q} \right)^i \Delta^i \gamma^p \Big|_{\gamma=n}.$$

Let us denote the first sum in expression (5.20) by K_3 and evaluate it. Then we obtain

$$K_3 = \sum_{\gamma=0}^{\beta-1} q^{\beta-\gamma} \gamma^3 = -\frac{q}{q-1} \left[\beta^3 + \frac{3\beta^2}{q-1} + \beta \frac{3(q+1)}{(q-1)^2} \right].$$

Next, let us denote the second sum in expression (5.20) by K_4 and compute it:

$$K_4 = \sum_{\gamma=0}^{\beta-1} q^{k-1-\beta+\gamma} \cdot \gamma^3 = q^{k-1-\beta} \cdot \sum_{\gamma=0}^{\beta-1} q^{\gamma} \cdot \gamma^3.$$

By applying formula (5.21) to this sum, we obtain

$$K_4 = -\frac{q^{k-1}}{1-q} \cdot \left(\beta^3 + \beta^2 \frac{3q}{1-q} + \beta \frac{3q(q+1)}{(1-q)^2} \right).$$

Thus, the sum S takes the following form:

$$\begin{aligned} S = K_1 - K_2 &= \frac{h^5}{6} \overset{\circ}{C}^{(\parallel)}[0] \beta^3 + \frac{h^5}{6} \left\{ a \frac{q}{1-q} \left(\beta^3 + \beta^2 \frac{3}{1-q} + \beta \frac{3(q+1)}{(1-q)^2} \right) \right. \\ &\quad \left. + b \frac{q^{k-1}}{q-1} \left(\beta^3 + \beta^2 \frac{3q}{1-q} + \beta \frac{3q(q+1)}{(1-q)^2} \right) \right\} \\ &\quad - \frac{h^5}{12} \beta^3 + \frac{h^5(k-1)}{4} \beta^2 - \frac{h^5}{4} \beta \sum_{\gamma=0}^{k-1} \overset{\circ}{C}^{(\parallel)}[\gamma] \gamma^2 + \frac{h^5}{12} \sum_{\gamma=0}^{k-1} \overset{\circ}{C}^{(\parallel)}[\gamma] \gamma^3. \end{aligned} \quad (5.22)$$

By adding $d_0 + d_1 \cdot [\beta]$ to expression (5.22) and collecting the terms of the left-hand side of equation (4.5) with respect to the powers of β , we obtain the following:

$$\begin{aligned} &\beta^3 h^5 \left[\frac{\overset{\circ}{C}^{(\parallel)}[0]}{6} - \frac{aq}{6(q-1)} + \frac{bq^{k-1}}{6(q-1)} - \frac{1}{12} \right] + \beta^2 h^5 \left(\frac{a}{12} + \frac{bq^{k-1}}{12} + \frac{k-1}{4} \right) \\ &+ \beta h^5 \left(\frac{a(q+1)}{12(q-1)} + \frac{bq^{k-1}(q+1)}{12(q-1)} \right) - \frac{1}{4} \sum_{\gamma=0}^{k-1} \overset{\circ}{C}^{(\parallel)}[\gamma] \gamma^2 + d_1 h^4 + \frac{h^5}{12} \sum_{\gamma=0}^{k-1} \overset{\circ}{C}^{(\parallel)}[\gamma] \gamma^3 + d_0. \end{aligned} \quad (5.23)$$

Now, by equating the coefficients of the powers of β in expression (5.23) with the coefficients of the powers of β on the right-hand side of equation (4.5), that is, in formula (5.3), we determine the values of a and b . First, let us rewrite formula (5.3) in terms of the powers of β :

$$-\frac{h^5}{12} \beta^3 + \frac{h^5(k-1)}{4} \beta^2 - \left(\frac{k^2}{4} - \frac{k}{2} - \frac{7}{24} \right) \beta + \frac{k^3}{12} - \frac{k^2}{4} + \frac{7k}{24} - \frac{1}{8}. \quad (5.24)$$

By equating the coefficients of β^3 and β^2 in expressions (5.23) and (5.24), we obtain the following system of equations:

$$\begin{cases} \frac{\overset{\circ}{C}^{(\parallel)}[0]}{6} - \frac{aq}{6(q-1)} + \frac{bq^{k-1}}{6(q-1)} - \frac{1}{12} = -\frac{1}{12}, \\ \frac{a}{12} + \frac{bq^{k-1}}{12} + \frac{k-1}{4} = \frac{k-1}{4}. \end{cases} \quad (5.25)$$

Solving the system (5.25), the values of a and b are obtained as follows:

$$a = -\frac{3q^{k-1}}{10(1-q^{2k-2})}, \quad (5.26)$$

$$b = \frac{3}{10(1-q^{2k-2})}. \quad (5.27)$$

Using the values of a and b , we can rewrite the coefficients $\overset{\circ}{C}^{(\parallel)}[\beta]$, $\beta = \overline{0, k-1}$ as follows:

$$\begin{aligned}\overset{\circ}{C}^{(II)}[0] &= \frac{3(1+q)q^{k-1}}{10(1-q^{2k-2})(1-q)}, \\ \overset{\circ}{C}^{(II)}[\beta] &= -\frac{3q^{k-1}}{10(1-q^{2k-2})}(q^\beta - q^{-\beta}), \quad \beta = \overline{1, k-3}, \\ \overset{\circ}{C}^{(II)}[k-2] &= \frac{1}{20} + \frac{3(q-q^{2k-3})}{10(1-q^{2k-2})}, \\ \overset{\circ}{C}^{(II)}[k-1] &= \frac{19}{20} - \frac{3(q+q^{2k-2})}{10(1-q)(1-q^{2k-2})}.\end{aligned}$$

Thus, **Theorem 5.1** is fully proved and **Problem 2.2** is also solved.

6. COMPUTATION OF THE NORM OF THE ERROR FUNCTIONAL OF THE EXPLICIT OPTIMAL DIFFERENCE FORMULA IN THE SOBOLEV SPACE $L_2^{(4)}(0,1)$

Theorem 6.1. *In the Sobolev space $L_2^{(4)}(0,1)$, the square of the norm of the error functional of the optimal explicit difference formula is expressed by the following formula:*

$$\|\ell|_{L_2^{(4)*}(0,1)}\|^2 = \left(\frac{421}{50400} - \frac{q+q^{2k-2}}{400(1-q)(1-q^{2k-2})} \right) h^7,$$

where $q = \sqrt{3} - 2$ is the root of the Euler polynomial of order two.

Proof. Initially, we determine the unknown coefficient d_1^- by equating expressions (5.16) and (5.26). Calculating the sum in (5.16), we obtain

$$a = \frac{A_2}{24q} (6(k-1)^2 + 1) + \frac{A_2}{h^4 q} d_1^-. \quad (6.1)$$

We equate (6.1) with (5.26):

$$\frac{A_2}{24q} (6(k-1)^2 + 1) + \frac{A_2}{h^4 q} d_1^- = -\frac{3q^{k-1}}{10(1-q^{2k-2})}. \quad (6.2)$$

From equation (6.2), we find d_1^- :

$$d_1^- = -\frac{3h^4 q^k}{10A_2(1-q^{2k-2})} - \frac{h^4}{24} (6(k-1)^2 + 1).$$

Now, we determine the coefficient d_1^+ by equating expressions (5.17) and (5.27). Here as well, if we first expand and simplify the sum in expression (5.17), it is equal to the following:

$$b = \frac{A_2}{20} + \frac{A_2(k-1)^2}{4q} - \frac{A_2}{h^4 q} d_1^+. \quad (6.3)$$

We equate (6.3) with (5.27):

$$\frac{A_2}{20} + \frac{A_2(k-1)^2}{4q} - \frac{A_2}{h^4 q} d_1^+ = \frac{3}{10(1-q^{2k-2})}. \quad (6.4)$$

From equation (6.4), we find d_1^+ :

$$d_1^+ = \frac{h^4 q}{120} + \frac{h^4 (k-1)^2}{4} - \frac{3h^4 q}{10A_2 (1-q^{2k-2})}.$$

Using the values of d_1^- and d_1^+ , we obtain d_1 :

$$d_1 = \frac{1}{2} (d_1^- + d_1^+) = \frac{1}{20} \left(\frac{q-5}{12} - \frac{3q}{A_2 (1-q^{k-1})} \right) h^4.$$

To determine d_0 , we need the explicit form of the unknown coefficient d_0^+ . Since d_0^- is known from formula (5.8), we have

$$d_0^+ = \frac{h^5}{120} - \frac{h^5 (k-1)^3}{12} - \frac{h^5 q (k-1)}{120} + \frac{3h^5 q (k-1)}{10A_2 (1-q^{2k-2})}.$$

Therefore

$$d_0 = \frac{1}{2} (d_0^- + d_0^+) = \left(\frac{1 + (k-1)(5-q)}{240} + \frac{3q(k-1)}{20A_2 (1-q^{2k-2})} \right) h^5.$$

In explicit form, according to **Theorem 3.2**, the square of the norm is given by the following:

$$\begin{aligned} \left\| \ell \Big|_{L_2^{(4)*}(0,1)} \right\|^2 &= \sum_{\beta=0}^k \sum_{\gamma=0}^k C[\beta] C[\gamma] G_3(h\beta - h\gamma) \\ &\quad - 2h^2 \sum_{\beta=0}^k \sum_{\gamma=0}^{k-1} C[\beta] C^{(\text{II})}[\gamma] G_4''(h\beta - h\gamma) + h^4 \sum_{\beta=0}^{k-1} \sum_{\gamma=0}^{k-1} C^{(\text{II})}[\beta] C^{(\text{II})}[\gamma] G_4^{IV}(h\beta - h\gamma). \end{aligned} \quad (6.5)$$

Now, let us compute (6.5):

$$\begin{aligned} \left\| \ell \Big|_{L_2^{(4)*}(0,1)} \right\|^2 &= \sum_{\beta=0}^k \sum_{\gamma=0}^k C[\beta] C[\gamma] G_3(h\beta - h\gamma) - h^2 \sum_{\gamma=0}^{k-1} \dot{C}^{(\text{II})}[\gamma] \left[\sum_{\beta=0}^k C[\beta] G_4''(h\beta - h\gamma) + d_0 + d_1[\beta] \right] \\ &= \sum_{\beta=0}^k \sum_{\gamma=0}^k C[\beta] C[\gamma] G_3(h\beta - h\gamma) - h^2 \sum_{\gamma=0}^{k-1} \dot{C}^{(\text{II})}[\gamma] [f_4[\beta] + d_0 + d_1[\beta]] = T_1 + T_2. \end{aligned}$$

where

$$\begin{aligned} T_1 &= \sum_{\beta=0}^k \sum_{\gamma=0}^k C[\beta] C[\gamma] G_3(h\beta - h\gamma), \\ T_2 &= -h^2 \sum_{\gamma=0}^{k-1} \dot{C}^{(\text{II})}[\gamma] [f_4[\beta] + d_0 + d_1[\beta]]. \end{aligned}$$

Now, let us compute T_1 and T_2 separately and then add them together. First, we compute T_1 :

$$T_1 = \sum_{\beta=0}^k \sum_{\gamma=0}^k C[\beta] C[\gamma] G_3(h\beta - h\gamma) = -8G_4(h) + 2G_4(2h) = -8\frac{h^7}{2 \cdot 7!} + 2\frac{(2h)^7}{2 \cdot 7!} = \frac{31}{1260}h^7.$$

Now, we calculate T_2 :

$$T_2 = -h^2 \sum_{\gamma=0}^{k-1} \dot{C}^{(\text{II})}[\gamma] [f_4[\gamma] + d_0 + d_1[\gamma]]$$

$$= -h^2 \overset{\circ}{C}^{(II)}[k-1]f_4[k-1] - h^2 \sum_{\gamma=0}^{k-2} \overset{\circ}{C}^{(II)}[\gamma]f_4[\gamma] - h^2 d_0 - h^3(k-1)d_1.$$

After simplification, we obtain

$$T_2 = -\frac{h^7}{5!} \overset{\circ}{C}^{(II)}[k-1] - h^2 d_0^+ - h^3(k-1)d_1^+ + \frac{h^7(k-1)^3}{6}. \quad (6.6)$$

Substituting $\overset{\circ}{C}^{(II)}[k-1]$, d_0^+ , and d_1^+ into (6.6), we have

$$T_2 = -\frac{39}{20 \cdot 5!} h^7 + \frac{3(q + q^{2k-2})}{10 \cdot 5! (1 - q^{2k-2})} h^7.$$

Now, adding T_1 and T_2 :

$$T_1 + T_2 = \frac{31}{1260} h^7 - \frac{39}{20 \cdot 5!} h^7 + \frac{3(q + q^{2k-2})}{10 \cdot 5! (1 - q^{2k-2})} h^7 = \left(\frac{421}{50400} - \frac{q + q^{2k-2}}{400(1-q)(1-q^{2k-2})} \right) h^7.$$

Therefore, the square of the norm is

$$\left\| \ell \right\|_{L_2^{(4)*}(0,1)}^2 = \left(\frac{421}{50400} - \frac{q + q^{2k-2}}{400(1-q)(1-q^{2k-2})} \right) h^7.$$

Thus, **Theorem 6.1** is completely proved.

7. CONCLUSION

In conclusion, it can be stated that in this work, the extremal function was derived for computing the norm of the error functional of the explicit optimal difference formula constructed for the approximate solution of second-order ordinary differential equations in the Sobolev space $L_2^{(4)}(0,1)$. Based on the obtained extremal function, an analytical expression for the square of the norm was established. To determine the optimal coefficients, the method of Lagrange multipliers was applied, and the corresponding Lagrangian function was constructed. By equating the partial derivatives of the Lagrangian with respect to the unknown variables to zero, a system of equations was obtained. This system was solved using the Sobolev method, yielding explicit forms of the optimal coefficients. Utilizing these coefficients, the square of the norm of the error functional was computed. Thus, an exact upper bound for the error of the constructed difference formula was established.

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