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Optimal Difference Formulas for an Approximate Solution of the Cauchy Problem

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Abstract. The key properties of numerical methods for solving ordinary differential equations are determined by their accuracy and stability. The step size is selected based on the accuracy of the numerical solution. In this paper, we will consider difference methods for the approximate solution of first-order ordinary differential equations. Here, we will find the square of the norm of the error functional of difference formulas. To obtain optimal coefficients, we will construct and analyze systems of linear algebraic equations. By solving this system, we will find the optimal coefficients of the difference formulas for specific spaces, and here we will calculate the square of the norm of the error functionals of the optimal difference formulas.

1. Introduction

The problem of solving ordinary differential equations is more complex than the problem of calculating single integrals, and accordingly the proportion of problems that can be integrated explicitly is significantly smaller here.

When explicit integrability is discussed, it is understood that the solution can be calculated using a finite number of elementary operations. In this sense, the class of explicitly integrable problems has come to include problems whose solutions are expressed through special functions. However, even this broader class represents a relatively small fraction of the problems presented for solution. A significant expansion of the class of actually solvable differential equations, and consequently an expansion of the scope of computational mathematics, occurred with the development of numerical methods and the active and collaborative use of computers.

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One of the simplest methods for solving the Cauchy problem, in terms of its formulation, is based on the Taylor formula.

Let a solution to a differential equation

$$y' = f(x, y) \tag{1.1}$$

on a segment $[x_0,\, x_0 + X]$ under the initial condition

$$y(x_0) = y_0, \tag{1.2}$$

where is $f(x, y)-$an analytic function.

For an approximate solution of the Cauchy problem (1.1)-(1.2) there are various methods, for example, the Euler method, the Adams method, the Adams-Bashforth method, the Runge-Kutta method, etc. ([1,2])

The numerical solution of ordinary differential equations (ODEs) has long been one of the key and, at the same time, most challenging problems in computational mathematics. Despite significant progress in algorithm development and computational technologies, obtaining stable and highly accurate numerical solutions for a wide class of ODEs still requires improved methods and in-depth analysis of their properties. Therefore, the problem of constructing efficient numerical schemes continues to be a focus of attention for many modern researchers.

In [3], S. Mehrkanoon, Z.A. Majid, M.Suleiman, K.I. Othman and Z.B. Ibrahim proposed an original approach to solving systems of first-order ordinary differential equations. The authors developed a numerical scheme based on the use of a three-point approximation and a three-step procedure, which allowed them to improve the accuracy of calculations and expand the scope of applicability of the method in solving complex dynamic systems.

In subsequent studies [4–6], the authors presented improved semi-explicit and semi-implicit versions of the predictor-corrector methods. The central focus of these studies was on analyzing the numerical stability of the proposed algorithms. By constructing stability regions, they demonstrated in detail the behavior of the methods for various integration steps and forms of the original problems. The analysis clearly demonstrated that semi-explicit schemes possess a significantly higher degree of stability compared to traditional predictor-corrector algorithms, making them preferable for solving stiff ODE systems and problems sensitive to the accumulation of numerical errors.

In this sense, the results of the mentioned studies make a significant contribution to the development of numerical integration methods and open up opportunities for creating more efficient and robust computational algorithms applicable in various areas of scientific and engineering problems.

Within this paper, we will construct optimal finite-difference formulas for the approximate solution of the Cauchy problem in specific functional spaces and will investigate the properties of these methods and estimates of their errors.

In the next section, we present an analytical expression for the square of the norm of the error functional and a system for finding the optimal coefficients of finite-difference formulas.

2. Optimization of finite difference formulas

Let us consider a difference formula of the form

$$\sum_{\beta=0}^{k} C[\beta]\varphi[\beta] - h\sum_{\beta=0}^{k} C^{(\mathrm{l})}[\beta]\varphi'[\beta] \cong 0 \tag{2.1}$$

Here $[\beta] = h\beta, h = \frac{1}{N}$, $N = 2, 3, ..., C[\beta]$ and $C^{(\mathrm{l})}[\beta]$ are the coefficients of the difference formula. The difference formula (2.1) is called implicit if $C^{(\mathrm{l})}[k] \neq 0$, and if $C^{(\mathrm{l})}[k] = 0$ then explicit.

We will consider the error of the difference formula as a linear functional of the form

$$\ell(x) = \sum_{\beta=0}^{k} C[\beta]\delta(x - h\beta) - h\sum_{\beta=0}^{k} C^{(\mathrm{l})}[\beta]\delta'(x - h\beta) \cong 0 \tag{2.2}$$

In the space $H_2^{(m)}(0,1)$ of classes of functions with derivatives of order m with an integrable square on a segment $[0,1]$ with a scalar product and a norm

$$(\psi, \varphi)_m = \sum_{n=0}^{m} \binom{m}{n} \int_0^1 \frac{d^n}{dx^n}\psi(x)\frac{d^n}{dx^n}\varphi(x), \tag{2.3}$$

$$\left\| f|H_2^{(m)}(0,1) \right\| = \left\{ \sum_{n=0}^{m} \binom{m}{n} \int_0^1 \left(\frac{d^n}{dx^n} f(x) \right)^2 dx \right\}^{\frac{1}{2}}, \tag{2.4}$$

where $\binom{m}{n} = \frac{m!}{(m-n)!n!}$.

The following theorem holds [7].

Theorem 2.1. *The square of the norm of the error functional of a difference formula of the k th order in space $H_2^{(m)}(0,1)$ is expressed by the formula*

$$\begin{aligned} \left\| \ell|H_2^{(m)*}(0,1) \right\|^2 = (-1)^m \Bigg[&\sum_{\beta=0}^{k}\sum_{\gamma=0}^{k} C[\beta]\ C[\gamma]\varepsilon_m(h\beta - h\gamma) - \\ &-2h\sum_{\beta=0}^{k} C^{(\mathrm{l})}[\beta]\sum_{\gamma=0}^{k} C[\gamma]\varepsilon'(h\beta - h\gamma) - \\ &-h^2\sum_{\beta=0}^{k}\sum_{\gamma=0}^{k} C^{(\mathrm{l})}[\beta]C^{(\mathrm{l})}[\gamma]\varepsilon''_m(h\beta - h\gamma) \Bigg]. \end{aligned} \tag{2.5}$$

Here

$$\varepsilon_m(x) = \frac{e^{-|x|}}{2^{2m-1}(m-1)!}\sum_{n=0}^{m-1} 2^n \frac{(2m-n-2)!\,|x|^n}{n!(m-n-1)!}, \tag{2.6}$$

$$\varepsilon'_m(x) = -signx\left[\varepsilon_m(x) - \frac{e^{-|x|}}{2^{2m-1}(m-1)!}\sum_{n=1}^{m-1} \frac{2^n(2m-n-2)!\,|x|^{n-1}}{(n-1)!(m-n-1)!} \right], \tag{2.7}$$

$$\varepsilon''_m(x) = \varepsilon_m(x) - \varepsilon_{m-1}(x). \tag{2.8}$$

The problem of constructing an optimal difference formula in a functional setting consists of finding a functional (2.2) whose norm in space $H_2^{(m)*}(0,1)$ is minimal.

It is known from [8,9] that the stability of the difference formula in the Dahlquist sense, as well as strong stability, is determined only by the coefficients $C[\beta]$, $\beta = 0,1,2, \dots, k$. Here we define these coefficients in the form

$$C[\beta] = \begin{cases} 1 \ for \ \beta = k, \\ -1 \ for \ \beta = k-1, \\ 0 \ for \ \beta = 0,1, \dots, k-2, \end{cases} \tag{2.9}$$

For this reason, our search for the optimal difference formula involves only changing the coefficients

$$C^{(l)}[\beta], \ \beta = 0\,,\,1\,, \dots, k.$$

By minimizing the square of the norm of the error functional (2.5) with respect to the coefficients, $C^{(l)}[\beta]$ we obtain the following theorem.

Theorem 2.2. *The optimal coefficients of the difference formula* (2.1) *in space* $H_2^{(m)}(0,1)$ *are determined from the following system*

$$h\sum_{\gamma=0}^{k} C^{(l)}[\beta]\varepsilon''_m(h\beta - h\gamma) = \varepsilon'_m(h\beta - h(k-1)) - \varepsilon'_m(h\beta - hk), \beta = 0,1, \dots, k. \tag{2.10}$$

Proof.

To prove the theorem, we denote by

$$\Phi\left(C^{(l)}\,(\beta)\right) = \left\| \ell | H_2^{(m)*}(0,1) \right\|^2.$$

To find the minimum of this function with respect to the coefficients $C^{(l)}[\beta]$, $\beta = 0\,,\,1\,, \dots, k$, we equate all partial derivatives with respect to $C^{(l)}[\beta]$ the function $\Phi\left(C^{(l)}\,(\beta)\right)$

$$\frac{\partial \Phi\left(C^{(l)}\,(\beta)\right)}{\partial C^{(l)}\,(\beta)} = 0$$

This gives a system of equations to find the optimal coefficients $\overset{\circ}{C}{}^{(l)}[\beta]$ for given $C[\beta]$.

$$h\sum_{\gamma=0}^{k} C^{(l)}[\beta]\varepsilon''_m(h\beta - h\gamma) = -\sum_{\gamma=0}^{k} C[\gamma]\varepsilon'_m(h\beta - hk), \beta = 0,1, \dots, k. \tag{2.11}$$

From this, using formula (2.9), we finally obtain

$$h\sum_{\gamma=0}^{k} C^{(l)}[\beta]\varepsilon''_m(h\beta - h\gamma) = \varepsilon'_m(h\beta - h(k-1)) - \varepsilon'_m(h\beta - hk), \beta = 0,1, \dots, k.$$

So, Theorem 2.2 is completely proven.

The solution of system (2.11), which we denote by $\overset{\circ}{C}^{(\mathrm{l})}[\beta]$, is a stationary point for the function $\Phi\left(C^{(\mathrm{l})}(\beta)\right)$.

Taking into account (2.11) for the optimal norm of the error functional, we obtain the following formula.

Theorem 2.3. *The square of the norm of the optimal error functional of the difference formula* (2.1) *has the form*

$$\left\|\overset{\circ}{\ell}|H_2^{(m)}\right\|^2 = (-1)^m\,[2(\varepsilon_m(0)-\varepsilon_m(h))+$$

$$\left.+h\sum_{\beta=0}^{k}\overset{\circ}{C}^{(\mathrm{l})}[\beta]\,(\varepsilon_m'(h\beta-h(k-1))-\varepsilon_m'(h\beta-hk))\right]. \tag{2.12}$$

Proof. To prove this theorem, we denote the second and third sums in formula (2.5) by

$$\mathrm{T}\left(C[\beta],\,C^{(\mathrm{l})}[\beta]\right) = -2h\sum_{\beta=0}^{k}C^{(\mathrm{l})}[\beta]\sum_{\gamma=0}^{k}C[\gamma]\varepsilon_m'(h\beta-h\gamma)-$$

$$-h^2\sum_{\beta=0}^{k}\sum_{\gamma=0}^{k}C^{(\mathrm{l})}[\beta]C^{(\mathrm{l})}[\gamma]\varepsilon_m''(h\beta-h\gamma). \tag{2.13}$$

Then, the square of the norm of the error functional (2.5) takes the following form

$$\left\|\ell|H_2^{(m)*}(0,1)\right\|^2 = (-1)^m\left[\sum_{\beta=0}^{k}\sum_{\gamma=0}^{k}C[\beta]C[\gamma]\varepsilon_m(h\beta-h\gamma)+\mathrm{T}\left(C[\beta],\,C^{(\mathrm{l})}[\beta]\right)\right]. \tag{2.14}$$

Now we transform the function $\mathrm{T}\left(C[\beta],\,C^{(\mathrm{l})}[\beta]\right)$ in the following form

$$\mathrm{T}\left(C[\beta],\,C^{(\mathrm{l})}[\beta]\right) = h\sum_{\beta=0}^{k}C^{(\mathrm{l})}[\beta]\left[-2\sum_{\gamma=0}^{k}C[\gamma]\varepsilon_m'(h\beta-h\gamma)-\ h\sum_{\beta=0}^{k}C^{(\mathrm{l})}[\beta]\varepsilon''(h\beta-h\gamma)\right]=$$

$$=h\sum_{\beta=0}^{k}C^{(\mathrm{l})}[\beta]\left[-\sum_{\gamma=0}^{k}C[\gamma]\varepsilon_m'(h\beta-h\gamma)-\left(\sum_{\gamma=0}^{k}C[\gamma]\varepsilon'(h\beta-h\gamma)\ +\right.\right.$$

$$\left.\left.+h\sum_{\gamma=0}^{k}C^{(\mathrm{l})}[\gamma]\varepsilon''(h\beta-h\gamma)\right)\right].$$

By (2.11), the last sums of the two expressions are equal to zero.
Then, we obtain

$$\mathrm{T}\left(C[\beta],\,C^{(\mathrm{l})}[\beta]\right) = -h\sum_{\beta=0}^{k}C^{(\mathrm{l})}[\beta]\sum_{\gamma=0}^{k}C[\gamma]\varepsilon_m'(h\beta-h\gamma)$$

Substituting this expression into (2.14), we obtain

$$\left\|\ell|H_2^{(m)*}(0,1)\right\|^2 = (-1)^m\left[\sum_{\beta=0}^{k}\sum_{\gamma=0}^{k}C[\beta]C[\gamma]\varepsilon_m(h\beta-h\gamma)-h\sum_{\beta=0}^{k}C^{(\mathrm{l})}[\beta]\sum_{\gamma=0}^{k}C[\gamma]\varepsilon_m'(h\beta-h\gamma)\right]$$

From here, $C[\beta]$ substituting the value according to formula (2.9) after some simplifications, we obtain the statement of Theorem 2.3.

It should be noted that optimization problems close to this topic can be found in the works [10–31].

3. Optimal coefficients of difference formulas

The main results of this section are the following theorems.

Theorem 3.1. *In the space, the $H_2^{(2)}(0,1)$ following $k=1$ explicit difference formula is optimal among difference formulas of the form* (2.1)

$$\varphi[1]-\varphi[0]=he^{-h}\varphi'[0].$$

Proof. Let $m=2$ and $k=1$.

In this case, for explicit difference formulas, system (2.10) takes the following form

$$h\overset{\circ}{C}{}^{(I)}[0]\varepsilon_2''(0)=\varepsilon_2'(0)-\varepsilon_2'(-h),$$

where

$$\varepsilon_2''(x)=\frac{e^{-|x|}}{4}\left(|x|-1\right), \tag{3.1}$$

$$\varepsilon_2'(x)=\frac{-xe^{-|x|}}{4}. \tag{3.2}$$

Using (3.1) and (3.2), we write equation (2.10) in the form $\frac{h}{4}\overset{\circ}{C}{}^{(I)}[0]=\frac{he^{-h}}{4}$, therefore

$$\overset{\circ}{C}{}^{(I)}[0]=e^{-h}. \tag{3.3}$$

From here in space $H_2^{(2)}(0,1)$ the optimal difference formula takes the form

$$\varphi[1]-\varphi[0]=he^{-h}\varphi'[0],$$

or

$$y_{n+1}=y_n+he^{-h}f(x_n,y_n). \tag{3.4}$$

So, we have obtained a one-step Euler-type method.

It is easy to see that

$$\lim_{h\to 0}\overset{\circ}{C}{}^{(I)}[0]=1.$$

Theorem 3.2. *Among all implicit difference formulas of the form* (2.1) *in the space $H_2^{(2)}(0,1)$ under $k=1$, there exists a unique implicit optimal difference formula, which takes the form*

$$\varphi[1]-\varphi[0]=\frac{h}{1-h+e^h}\left(\varphi'[0]+\varphi'[1]\right)$$

Proof. Let $m = 2$ and $k = 1$.

In this case, for implicit difference formulas, system (2.10) takes the following form

$$\begin{cases} h\overset{\circ}{C}{}^{(l)}[0]\varepsilon_2''(0) + h\overset{\circ}{C}{}^{(l)}[1]\varepsilon_2'(-h) = \varepsilon_2'(0) - \varepsilon_2'(-h) \\ h\overset{\circ}{C}{}^{(l)}[0]\varepsilon_2''(h) + h\overset{\circ}{C}{}^{(l)}[1]\varepsilon_2'(0) = \varepsilon_2'(h) - \varepsilon_2'(0) \end{cases}$$

By formulas (3.1) and (3.2) and after some simplifications, we reduce this system to the following form

$$\begin{cases} -\overset{\circ}{C}{}^{(l)}[0] + \overset{\circ}{C}{}^{(l)}[1]e^{-h}(h-1) = -e^{-h} \\ \overset{\circ}{C}{}^{(l)}[0]e^{-h}(h-1) - \overset{\circ}{C}{}^{(l)}[1] = -e^{-h} \end{cases}$$

It immediately follows that

$$\overset{\circ}{C}{}^{(l)}[0] = \overset{\circ}{C}{}^{(l)}[1]$$

Then, from the first equation, we obtain

$$\overset{\circ}{C}{}^{(l)}[0] = \frac{1}{1-h+e^h}, \tag{3.5}$$

$$\overset{\circ}{C}{}^{(l)}[1] = \frac{1}{1-h+e^h}, \tag{3.6}$$

In this case, i.e. for $m = 2$ and $k = 1$ the optimal implicit difference formula of form (2.1) takes the following form:

$$\varphi[1] - \varphi[0] = \frac{h\varphi'[0]}{1-h+e^h} + \frac{h\varphi'[1]}{1-h+e^h}$$

or

$$y_{n+1} = y_n + \frac{h}{1-h+e^h}\left(f(x_n, y_n) + f(x_{n+1}, y_{n+1})\right).$$

It is easy to see that

$$\lim_{h\to 0}\overset{\circ}{C}{}^{(l)}[0] = \frac{1}{2}$$

$$\lim_{h\to 0}\overset{\circ}{C}{}^{(l)}[1] = \frac{1}{2}$$

So, in $h \to 0$ $\overset{\circ}{C}{}^{(l)}[0] + \overset{\circ}{C}{}^{(l)}[1]$ tends to one.

Theorem 3.3. *In the space $H_2^{(2)}(0, 1)$ at $k = 2$ the following explicit difference formula of the form* (2.1) *is optimal*

$$\varphi[2] - \varphi[1] = \frac{h\left(1+h-e^h\right)\varphi'[0]}{e^{2h}-(h-1)^2} + \frac{h\left(e^h+(h-1)\left(2e^{-h}-1\right)\right)\varphi'[1]}{e^{2h}-(h-1)^2}.$$

Proof. Let $m = 2$ and $k = 2$.

Then system (2.10) for the optimal coefficients of explicit difference formulas takes the form

$$\begin{cases} h\overset{\circ}{C}{}^{(l)}[0]\varepsilon_2''(0) + h\overset{\circ}{C}{}^{(l)}[1]\varepsilon_2''(-h) = \varepsilon_2'(-h) - \varepsilon_2'(-2h) \\ h\overset{\circ}{C}{}^{(l)}[0]\varepsilon_2''(h) + h\overset{\circ}{C}{}^{(l)}[1]\varepsilon_2''(0) = \varepsilon_2'(0) - \varepsilon_2'(-h) \end{cases}$$

From here, using the formulas for $\varepsilon_2''(x)$ and $\varepsilon_2'(x)$ using the given formulas (3.1) and (3.2) we obtain

$$\begin{cases} \overset{\circ}{C}{}^{(l)}[0] + e^{-h}(h-1)\overset{\circ}{C}{}^{(l)}[1] = 2e^{-2h} - e^{-h} \\ e^{-h}(h-1)\overset{\circ}{C}{}^{(l)}[0] - \overset{\circ}{C}{}^{(l)}[1] = -e^{-h} \end{cases}$$

Solving this system, we have

$$\overset{\circ}{C}{}^{(l)}[0] = \frac{1+h-e^h}{e^{2h}-(h-1)^2}, \tag{3.7}$$

$$\overset{\circ}{C}{}^{(l)}[1] = \frac{e^h + (h-1)(2e^{-h}-1)}{e^{2h}-(h-1)^2}. \tag{3.8}$$

So, we have proved that in the space $H_2^{(2)}(0,1)$ for, $k=2$ the explicit optimal difference formula of the form (2.1) has the following form:

$$\varphi[2] - \varphi[1] = \frac{h\left(1+h-e^h\right)\varphi'[0]}{e^{2h}-(h-1)^2} + \frac{h\left(e^h + (h-1)\left(2e^{-h}-1\right)\right)\varphi'[1]}{e^{2h}-(h-1)^2}.$$

or

$$y_{n+2} = y_{n+1} + \frac{h\left(1+h-e^h\right)}{e^{2h}-(h-1)^2} f\left(x_n, y_n\right) + \frac{h\left(e^h + (h-1)\left(2e^{-h}-1\right)\right)}{e^{2h}-(h-1)^2} f\left(x_{n+1}, y_{n+1}\right).$$

It is not difficult to show that

$$\lim_{h\to 0}\overset{\circ}{C}{}^{(l)}[0] = \lim_{h\to 0}\frac{1+h-e^h}{e^{2h}-(h-1)^2} = 0$$

$$\lim_{h\to 0}\overset{\circ}{C}{}^{(l)}[1] = \lim_{h\to 0}\frac{e^h + (h-1)(2e^{-h}-1)}{e^{2h}-(h-1)^2} = 1$$

So, $\overset{\circ}{C}{}^{(l)}[0] + \overset{\circ}{C}{}^{(l)}[1]$ tends to one as $h \to 0$.

Theorem 3.4. *In the space $H_2^{(2)}(0,1)$ when $k=2$ the optimal implicit difference formula is defined by the equality*

$$\varphi[2] - \varphi[1] = h\left(\overset{\circ}{C}{}^{(l)}[0][0]\varphi'[0] + \overset{\circ}{C}{}^{(l)}[1]\varphi'[1] + \overset{\circ}{C}{}^{(l)}[2]\varphi'[2]\right).$$

Here

$$\overset{\circ}{C}{}^{(l)}[0] = \frac{e^{2h}(e^h-h-1) - e^h(2h^2-2h+1) + 1 - h}{-e^{4h} + 2e^{2h}(h-1)^2 + 4h^3 - 6h^2 + 4h - 1},$$

$$\overset{\circ}{C}{}^{(l)}[1] = \frac{-e^{3h} - 2e^h(h-1) + e^{-h}(2h-1)}{-e^{4h} + 2e^{2h}(h-1)^2 + 4h^3 - 6h^2 + 4h - 1},$$

$$\overset{\circ}{C}{}^{(l)}[2] = \frac{-e^{2h}(e^h+h-1) + e^h(2h^2-2h+1) - 4h^2 + 3h - 1}{-e^{4h} + 2e^{2h}(h-1)^2 + 4h^3 - 6h^2 + 4h - 1}.$$

Proof. Let $m = 2, k = 2$.

In this case, system (2.10) for implicit difference formulas has the form

$$\begin{cases} h\overset{\circ}{C}^{(l)}[0]\varepsilon_2''(0) + h\overset{\circ}{C}^{(l)}[1]\varepsilon_2''(-h) + h\,\overset{\circ}{C}^{(l)}[2]\varepsilon_2''(-2h) = \varepsilon_2'(-h) - \varepsilon_2'(-2h), \\ h\overset{\circ}{C}^{(l)}[0]\varepsilon_2''(h) + h\overset{\circ}{C}^{(l)}[1]\varepsilon_2''(0) + h\overset{\circ}{C}^{(l)}[2]\varepsilon_2''(-h) = \varepsilon_2'(0) - \varepsilon_2'(-h), \\ h\overset{\circ}{C}^{(l)}[0]\varepsilon_2''(2h) + h\overset{\circ}{C}^{(l)}[1]\varepsilon_2''(h) + h\overset{\circ}{C}^{(l)}[2]\varepsilon_2''(0) = \varepsilon_2'(h) - \varepsilon_2'(0). \end{cases}$$

This system, by formulas (3.1) and (3.2), takes the following form

$$\begin{cases} -e^h\overset{\circ}{C}^{(l)}[0] + (h-1)\overset{\circ}{C}^{(l)}[1] + e^{-h}(2h-1)\overset{\circ}{C}^{(l)}[2] = 1 - 2e^{-h}, \\ (h-1)\overset{\circ}{C}^{(l)}[0] - e^h\overset{\circ}{C}^{(l)}[1] + (h-1)\overset{\circ}{C}^{(l)}[2] = -1, \\ e^{-h}(2h-1)\overset{\circ}{C}^{(l)}[0] + (h-1)\overset{\circ}{C}^{(l)}[1] - e^h\overset{\circ}{C}^{(l)}[2] = -1. \end{cases}$$

We solve this system using Cramer's method.

To do this, by calculating the determinants $\Delta,\ \Delta_1,\ \Delta_2,\ \Delta_3$, we find the optimal coefficients $\overset{\circ}{C}^{(l)}[0]$, $\overset{\circ}{C}^{(l)}[1]$, $\overset{\circ}{C}^{(l)}[2]$,

$$\Delta = \begin{vmatrix} -e^h & h-1 & (2h-1)e^{-h} \\ (h-1) & -e^h & h-1 \\ (2h-1)e^{-h} & h-1 & -e^h \end{vmatrix} = -e^{3h} + e^{-h}(4h^3 - 6h^2 + 4h - 1) + 2e^h(h-1)^2,$$

$$\Delta_1 = \begin{vmatrix} 1-2e^{-h} & h-1 & (2h-1)e^{-h} \\ -1 & -e^h & h-1 \\ -1 & h-1 & -e^h \end{vmatrix} = e^h(e^h - h - 1) + h(1-2h) + (h-1)(1-e^{-h}),$$

$$\Delta_2 = \begin{vmatrix} -e^h & 1-2e^h & (2h-1)e^{-h} \\ h-1 & -1 & h-1 \\ (2h-1)e^{-h} & -1 & -e^h \end{vmatrix} = -e^{2h} - 2(h-1) + e^{-2h}(2h-1),$$

$$\Delta_3 = \begin{vmatrix} -e^h & h-1 & 1-2e^{-h} \\ h-1 & -e^h & -1 \\ (2h-1)e^{-h} & h-1 & -1 \end{vmatrix} = -e^h(e^h + h - 1) - e^{-h}(4h^2 - 3h + 1) + 2h^2 - 2h + 1.$$

Then, the optimal coefficients take the form

$$\overset{\circ}{C}^{(l)}[0] = \frac{e^h(e^h - h - 1) + h(1-2h) + (h-1)(1-e^{-h})}{-e^{3h} + e^{-h}(4h^3 - 6h^2 + 4h - 1) + 2e^h(h-1)^2} =$$

$$= \frac{e^{2h}(e^h - h - 1) - e^h(2h^2 - h) + (h-1)(e^h - 1)}{-e^{4h} + 2e^{2h}(h-1)^2 + 4h^3 - 6h^2 + 4h - 1} =$$

$$= \frac{e^{2h}(e^h - h - 1) - e^h(2h^2 - h + 1 - h) + 1 - h}{-e^{4h} + 2e^{2h}(h-1)^2 + 4h^3 - 6h^2 + 4h - 1} \tag{3.9}$$

$$\overset{\circ}{C}^{(l)}[1] = \frac{-e^{3h} - 2e^h(h-1) + e^{-h}(2h-1)}{-e^{4h} + 2e^{2h}(h-1)^2 + 4h^3 - 6h^2 + 4h - 1}, \tag{3.10}$$

$$\overset{\circ}{C}{}^{(\mathrm{I})}[2]=\frac{-e^{2h}(e^h+h-1)+e^h(2h^2-2h+1)-4h^2+3h-1}{-e^{4h}+2e^{2h}(h-1)^2+4h^3-6h^2+4h-1}. \tag{3.11}$$

Thus, in the space $H_2^{(2)}(0,\,1)$ when $k=2$ the optimal implicit difference formula is determined by the formula

$$\varphi[2]-\varphi[1]=h\overset{\circ}{C}{}^{(\mathrm{I})}[0][0]\varphi'[0]+h\overset{\circ}{C}{}^{(\mathrm{I})}[1]\varphi'[1]+h\overset{\circ}{C}{}^{(\mathrm{I})}[2]\varphi'[2],$$

where $\overset{\circ}{C}{}^{(\mathrm{I})}[0]$, $\overset{\circ}{C}{}^{(\mathrm{I})}[1]$, $\overset{\circ}{C}{}^{(\mathrm{I})}[2]$ are defined by equalities (3.9), (3.10), (3.11),
or

$$y_{n+2}=y_{n+1}+h\overset{\circ}{C}{}^{(\mathrm{I})}[0]f\left(x_n,\,y_n\right)+h\overset{\circ}{C}{}^{(\mathrm{I})}[1]f\left(x_{n+1},\,y_{n+1}\right)+h\overset{\circ}{C}{}^{(\mathrm{I})}[2]f\left(x_{n+2},\,y_{n+2}\right).$$

It is not difficult to see that

$$\lim_{h\to 0}\overset{\circ}{C}{}^{(\mathrm{I})}[0]=0,\lim_{h\to 0}\overset{\circ}{C}{}^{(\mathrm{I})}[1]=\frac{1}{2},\lim_{h\to 0}\overset{\circ}{C}{}^{(\mathrm{I})}[2]=\frac{1}{2}.$$

From this it is clear that

$$\lim_{h\to 0}\left(\overset{\circ}{C}{}^{(\mathrm{I})}[0]+\overset{\circ}{C}{}^{(\mathrm{I})}[1]+\overset{\circ}{C}{}^{(\mathrm{I})}[2]\right)=1.$$

4. The square of the norm of optimal error functionals

To calculate the square of the norm of optimal difference formulas, we will use formula (2.12).

a) Let $m=2$, $k=1$ and let us consider the optimal error functional for explicit difference formulas.

Using formulas (2.6), (2.12), (3.2) and (3.3) after some simplifications, we have

$$\left\|\overset{\circ}{\ell}|H_2^{(2)*}(0,1)\right\|^2=\frac{3-2e^{-h}-(1+he^{-h})^2}{4}. \tag{4.1}$$

Expanding the right side of formula (2.5) in powers, h we have

$$\left\|\overset{\circ}{\ell}|H_2^{(2)*}(0,1)\right\|^2=\frac{h^3}{3}-\frac{7h^4}{16}+\frac{19}{60}h^5-\frac{47}{288}h^6+\frac{37}{560}h^7+O(h^8). \tag{4.2}$$

b) Let $m=2$, $k=1$. Let us consider the square of the norm of the error functional of optimal implicit difference formulas.

Substituting the expressions for $\varepsilon_2(x)$ and $\varepsilon_2'(x)$ given by formulas (2.6), (3.2), (3.6), (3.7) into (2.12), after some calculations, we obtain

$$\left\|\overset{\circ}{\ell}|H_2^{(2)*}(0,1)\right\|^2=\frac{e^h-e^{-h}-2h}{2(1-h+e^h)}. \tag{4.3}$$

From this, expanding by h, we obtain

$$\left\|\overset{\circ}{\ell}|H_2^{(2)*}(0,1)\right\|^2=\frac{h^3}{12}-\frac{h^5}{60}-\frac{h^6}{144}+\frac{17}{6720}h^7+O(h^8). \tag{4.4}$$

c) Let $m=2$, $k=2$.

In this case, the square of the norm of the error functional of optimal explicit difference formulas, taking into account formulas (2.6), (2.12), (3.2), (3.7), (3.8), takes the following form

$$\left\|\overset{\circ}{\ell}|H_2^{(2)*}(0,1)\right\|^2 = \frac{1-e^{-h}(1+h)}{2} - \frac{h^2e^{-2h}}{4}\left(1+\frac{\left(e^h-h-1\right)^2}{e^{2h}-(h-1)^2}\right). \tag{4.5}$$

In this case, expanding the right-hand side of (4.5) we $h$have

$$\left\|\overset{\circ}{\ell}|H_2^{(2)*}(0,1)\right\|^2 = \frac{h^3}{3} - \frac{7}{16}h^4 + \frac{3h^5}{10} - \frac{319}{2304}h^6 + \frac{16237}{322560}h^7 + O(h^8) \tag{4.6}$$

d) Let $m=2$, $k=2$.

Then, by virtue of formulas (2.6), (2.12), (3.2), (3.9), (3.10), (3.11), the square of the norm of the error functional of optimal implicit difference formulas is expressed by the formula

$$\left\|\overset{\circ}{\ell}|H_2^{(2)*}(0,1)\right\|^2 = \frac{1}{2}\left(1-e^{-h}(1+h)\right) -$$

$$-\frac{h^2\left[-3e^{2h}+4e^h-e^{-h}(8h^2-8h+4)+e^{2h}+4h^2-8h+2\right]}{4\left[-e^{4h}+2e^{2h}(h-1)^2+4h^3-6h^2+4h-1\right]} \tag{4.7}$$

From here, expanding the right-hand side of (4.7) by h we obtain

$$\left\|\overset{\circ}{\ell}|H_2^{(2)*}(0,1)\right\|^2 = \frac{h^3}{12} - \frac{h^5}{60} - \frac{h^6}{144} + \frac{h^7}{1260} + O(h^8). \tag{4.8}$$

In the work [11, 12], it is proved that in space $L_2^{(2)}(0,1)$, the following Euler formula $y_{n+1} = y_n + hf(x_n, y_n)$ is an optimal difference formula. In this case, the square of the norm of the error functional of the Euler difference formula has the form

$$\left\|\overset{\circ}{\ell}|L_2^{(2)}(0,1)\right\|^2 = \frac{h^3}{3}. \tag{4.9}$$

From (4.2) and (4.9) it is evident that the error of the optimal difference formula (3.4), tends to zero faster than the Euler formula.

5. Numerical results

In this section, we present some numerical results showing in the form of tables and graphs the approximate solutions of our optimal explicit and implicit difference formulas given in Theorem 4 and Theorem 5, respectively.

```
Example: y'=np.exp(x-w), N = 10, h = 0.1, y_0=0; exact solution: y(x)=np.log(np.exp(x)+np.exp(1)-1)-1
N=10
y_0=0
```

t	Exact solution	Solution of the Euler Method	Error of the Euler Method	Solution of the Optimal exp.diff. formula	Error of the Optimal exp.dif f.formula
0.0	0.0	0.0	0.0	0.0	0.0
0.1	0.037960514214082	0.1	0.062039485785918	0.090483741803596	0.052523227589514
0.2	0.078302292132456	0.2	0.121697707867544	0.181832660350277	0.103530368217821
0.3	0.12107172210077	0.3	0.17892827789923	0.273975274042569	0.152903551941799
0.4	0.166304122292324	0.4	0.233695877707676	0.366844739684764	0.200540617392439
0.5	0.214023060629709	0.5	0.285976939370291	0.460378780815856	0.246355720186147
0.6	0.264239892733616	0.6	0.335760107266384	0.554519568695569	0.290279675961954
0.7	0.316953536942687	0.7	0.383046463057313	0.649213566525205	0.332260029582518
0.8	0.372150495809544	0.8	0.427849504190455	0.744411346264858	0.372260850455314
0.9	0.429805123170661	0.9	0.470194876829339	0.840067386163554	0.410262262992892
1.0	0.48988012564475	1.0	0.51011987435525	0.936139855905494	0.446259730260745

FIGURE 1. The table presents exact solutions and approximate solutions using explicit formulas, as well as their errors.

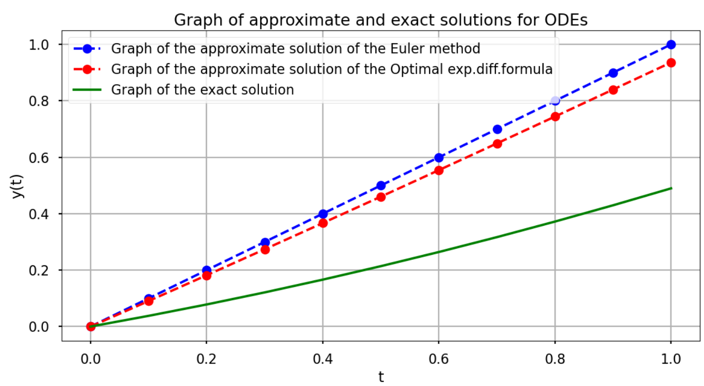

FIGURE 2. The figure shows a graphical representation of solutions obtained using explicit Euler formulas and optimal explicit difference formulas.

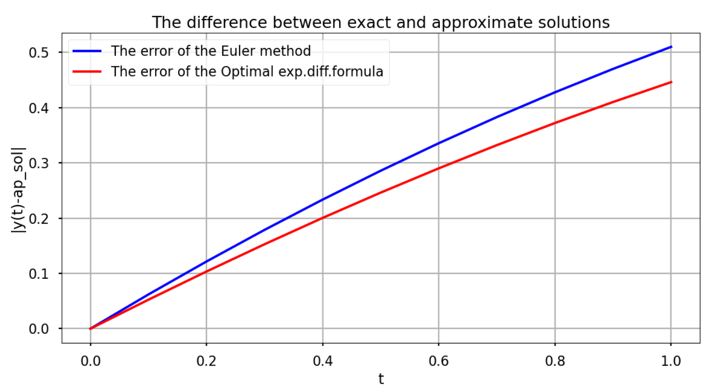

FIGURE 3. The figure clearly illustrates the difference between exact and approximate solutions.

```
Example: y'=np.exp(x-w), N = 10, h = 0.1, y_0=0; exact solution: y(x)=np.log(np.exp(x)+np.exp(1)-1)-1
N=10
y_0=0
```

t	Exact solution	Solution of the Euler implicit Method	Error of the Euler implicit Method	Solution of the Optimal imp. diff.formula	Error of the Optimal imp. diff.formula
0.0	0.0	0.0	0.0	0.0	0.0
0.1	0.037960514214082	0.1	0.062039485785918	0.090483741803596	0.052523227589514
0.2	0.078302292132456	0.2	0.121697707867544	0.181832660350277	0.103530368217821
0.3	0.12107172210077	0.3	0.17892827789923	0.273975274042569	0.152903551941799
0.4	0.166304122292324	0.4	0.233695877707676	0.366844739684764	0.200540617392439
0.5	0.214023060629709	0.5	0.285976939370291	0.460378780815856	0.246355720186147
0.6	0.264239892733616	0.6	0.335760107266384	0.554519568695569	0.290279675961954
0.7	0.316953536942687	0.7	0.383046463057313	0.649213566525205	0.332260029582518
0.8	0.372150495809544	0.8	0.427849504190455	0.744411346264858	0.372260850455314
0.9	0.429805123170661	0.9	0.470194876829339	0.840067386163554	0.410262262992892
1.0	0.48988012564475	1.0	0.51011987435525	0.936139855905494	0.446259730260745

FIGURE 4. The table presents exact solutions and approximate solutions using implicit formulas, as well as their errors.

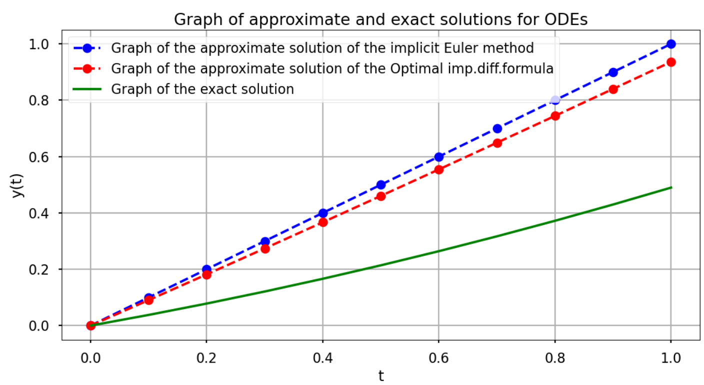

FIGURE 5. The figure shows a graphical representation of solutions obtained using implicit Euler formulas and optimal explicit difference formulas.

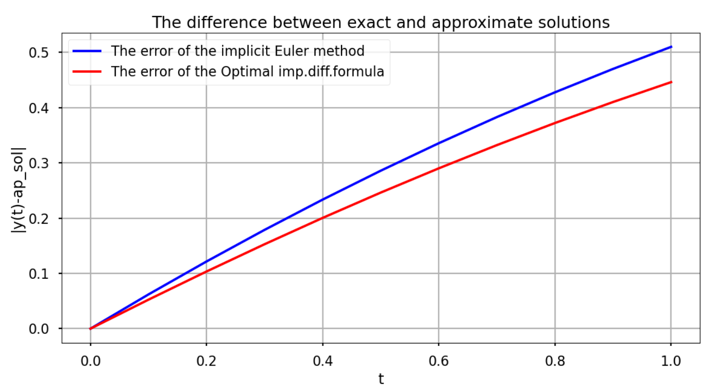

FIGURE 6. The figure clearly illustrates the difference between exact and approximate solutions.

Conclusion

In this paper, we considered the problem of constructing optimal difference formulas and estimating their errors in various functional spaces. Here, for any m expressions for the square of the norm of the error functional of optimal difference formulas were obtained. For $m = 2$ and $k = 1, 2$ optimal coefficients were found for explicit and implicit difference formulas. In these cases, the square of the norm of the error functional of optimal difference formulas was explicitly found. Furthermore, an expansion of the expression for the square of the norm of optimal difference formulas in grid steps is presented.

Conflicts of Interest: The authors declare that there are no conflicts of interest regarding the publication of this paper.

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