METHOD OF FUNCTION EXTRAPOLATION USING GODUNOV REGULARIZATION OF ILL-CONDITIONED SLAES

E.A. BIBERDORF AND K.K. ABDISHERIPOV

Abstract: This article proposes a new, original numerical method for function extrapolation. The method is based on the fact that at grid points on an interval where the function is known, the conditions for its coincidence with the extrapolating function are represented as an underdetermined linear system. This system is regularized by adding grid smoothness conditions. The values of the extrapolating function at grid points are found as pseudo-solutions of the extended system. The extrapolation is shown to be polynomial. Condition estimates for the regularized system are obtained. Numerous tests have confirmed the effectiveness of the method.

Keywords: extrapolation, finite differences, ill-conditioned SLAEs, regularization, least squares method.

1 Introduction

Extrapolation methods occupy an important place in numerical analysis, since they allow one to reconstruct the behavior of a function where direct measurements or calculations are impossible, based on known values over a given interval. Typically, interpolation polynomials constructed from known function values are used for extrapolation. This paper describes an original approach based on a method for regularizing ill-conditioned linear equations, proposed in the 1980s by Sergei Konstantinovich Godunov [1]-[3].

S.K. Godunov's scientific approach was deeply practical. He emphasized that any mathematical problem must be analyzed taking into account its physical content, and if a mathematical problem is ill-conditioned, it means that not all physical aspects were taken into account when it was formulated.

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Applying this methodological principle to the problem of ill-conditioned linear equations, S.K. Godunov proposed expanding such systems using equations that reflect some additional a priori information about the solution, such as its smoothness. A weighting parameter can be used to balance the inaccuracies in the specification of the primary and auxiliary subsystems. This means that such regularization does not increase the level of solution error.

This approach has proven effective in other problems as well. It was previously used in the paper [4] as the basis for a new hybrid method of approximation, interpolation, and smoothing. There, the effectiveness of combining the basic system with regularizing conditions of difference smoothness in processing discrete data was demonstrated for the first time. In this paper, we use the same mechanism for extending the system using difference smoothness operators, but now apply it not to approximation and interpolation within an interval, but to recovering values beyond it. Thus, this paper is a natural extension of our previously proposed methodology.

2 Description of the method

Consider a function $f(x)$ defined on the interval $[a,b]$ at the nodes of a uniform grid:

$$a = x_1 < x_2 < \cdots < x_{n_1} = b, \qquad x_{j+1} = x_j + h, \qquad j = 1, \ldots, n_1 - 1,$$

where h is a fixed grid step. It is necessary to recover approximate values of the function on the interval $(b,c]$, which extends beyond the domain of known data, at the points

$$b+h = x_{n_1+1} < x_{n_1+2} < \cdots < x_{n_2} = c, \qquad x_{j+1} = x_j+h, \qquad j = n_1+1, \ldots, n_2-1.$$

We will call the intervals $[a,b]$ and $(b,c]$ the interpolation and extrapolation intervals, respectively. We will denote the total number of nodes by $n = n_1 + n_2$, and the desired approximation by $g(x)$. We will also introduce notations for vectors containing given and sought values:

$$f = \begin{pmatrix} f(x_1) \\ \vdots \\ f(x_{n_1}) \end{pmatrix}, \quad g_1 = \begin{pmatrix} g(x_1) \\ \vdots \\ g(x_{n_1}) \end{pmatrix}, \quad g_2 = \begin{pmatrix} g(x_{n_1+1}) \\ \vdots \\ g(x_{n_2}) \end{pmatrix}, \quad g = \begin{pmatrix} g_1 \\ g_2 \end{pmatrix}.$$

The condition of equality of the functions $f(x)$ and $g(x)$ on the interpolation interval $[a,b]$ means the equality of the vectors $g_1 = f$, which implies the system

$$Bg = f, \tag{1}$$

where the matrix B has the form:

$$B = \begin{bmatrix} I_{n_1} & O \end{bmatrix}.$$

Here I_{n_1} is the identity matrix $n_1 \times n_1$, and O is a zero matrix of suitable size. Thus, the matrix B selects the first n_1 components of the vector g corresponding to the known values of the function $f(x)$ on the interpolation interval $[a, b]$. This system is clearly underdetermined. To solve it, we apply Godunov regularization. To this end, the system is supplemented with zero-valued finite differences of fixed order:

$$\sum_{k=0}^{p}(-1)^k C_p^k g(x_{j+k}) = 0, \quad j = 1, \dots, n-p-1. \tag{2}$$

This additional system can be interpreted in two ways. First, we can assume that the desired function $g(x)$ is sufficiently smooth and its divided differences are bounded

$$\frac{\left|\sum_{k=0}^{p}(-1)^k C_p^k g(x_{j+k})\right|}{h^p} < C,$$

and therefore the finite differences are close to zero:

$$\left|\sum_{k=0}^{p}(-1)^k C_p^k g(x_{j+k})\right| < h^p C \approx 0.$$

In this case, the additional equations are satisfied with an accuracy of $h^p C$.

Secondly, we can assume that the extrapolation is performed by a polynomial of degree no greater than $p-1$, then the additional equations (2) are satisfied exactly.

If we denote D_p as the finite difference matrix of order p, then the system of equations (2) takes the form $D_p g = 0$. Combining equations (1) and (2) yields a system of the form:

$$Ag \approx b, \quad A = \begin{pmatrix} B \\ \dots \\ D_p \end{pmatrix}, \quad b = \begin{pmatrix} f \\ \dots \\ O \end{pmatrix}. \tag{3}$$

The combined system is overdetermined but has full rank, so it has a unique pseudo-solution that minimizes the residual: $\|Ag - b\|_2$. We will choose this pseudo-solution as the desired extrapolation.

3 Properties of the system and solutions

To calculate a pseudo-solution to the overdetermined regularized problem (3), it is necessary to apply the least-squares method. The growth of the condition number depending on the order p and the total number of points n is described by the following theorem.

Theorem 1. *Let $p+1 < n_1$, then the condition number of the matrix A (3) satisfies the estimate*

$$cond\,(A) \leq (4n)^p. \tag{4}$$

Proof. Together with the rectangular matrix A, we consider the square lower triangular matrix

$$A_0 = \begin{bmatrix} I_p & O \\ & B \end{bmatrix}.$$

Then, up to a permutation of rows, the matrix A is a one-sided bordering of the matrix A_0. Therefore, by the one-sided bordering theorem [5], the following relations hold between their singular values

$$\sigma_{\min}(A_0) \le \sigma_{\min}(A).$$

Next, in order to estimate $\sigma_{\min}(A_0)$, we represent this matrix as a product

$$A_0 = \begin{bmatrix} I_p & O \\ & B \end{bmatrix} = \begin{bmatrix} R_p^{-1} & O \\ O & I_n \end{bmatrix} R_n,$$

where the matrices R_k are lower triangular Toeplitz matrices of size $k \times k$, composed of binomial coefficients:

$$R_k = \begin{bmatrix} (-1)^p C_p^p & 0 & \dots & \dots & \dots & \dots & 0 \\ (-1)^{p-1} C_p^{p-1} & (-1)^p C_p^p & 0 & \dots & & \dots & 0 \\ \vdots & \ddots & \ddots & \ddots & & & \vdots \\ C_p^0 & & \ddots & \ddots & \ddots & & \vdots \\ 0 & \ddots & & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & & \ddots & (-1)^p C_p^p & 0 \\ 0 & \dots & 0 & C_p^0 & \dots & (-1)^{p-1} C_p^{p-1} & (-1)^p C_p^p \end{bmatrix}. \tag{5}$$

Note that these matrices in turn are powers of matrices of a simpler structure:

$$R_k = J_k^p = \begin{bmatrix} -1 & 0 & \dots & \dots & 0 \\ 1 & -1 & \ddots & & \vdots \\ 0 & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & -1 & 0 \\ 0 & \dots & 0 & 1 & -1 \end{bmatrix}^p .$$

It is easy to check that the inverse matrices have the form

$$J_k^{-1} = -\begin{bmatrix} 1 & 0 & \dots & 0 \\ 1 & 1 & & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 1 & \dots & 1 & 1 \end{bmatrix}.$$

From the obvious estimates $\|J_k\| \le 2$, $\|J_k^{-1}\| \le k$ it follows that $\|R_k\| \le 2^p$, $\|R_k^{-1}\| \le k^p$, and therefore

$$\sigma_{\min}(A) \ge \sigma_{\min}(A_0) \ge \sigma_{\min}(R_p^{-1})\sigma_{\min}(R_n) \ge \frac{1}{(2n)^p}. \tag{6}$$

For the norm of the matrix A the following estimate holds:

$$\sigma_{\max}(A) = \|A\| \le \sum_{j=0}^{p} C_p^j = 2^p. \tag{7}$$

Substituting the estimates (6), (7) into the fraction $\mathrm{cond}\,(A) = \sigma_{\max}(A)/\sigma_{\min}(A)$ completes the proof. □

Theorem 2. *If g is a pseudo-solution of the system (3), then the points (x_j, g_j), $n_1 + 1 \le j \le n$, belong to the graph of a polynomial of degree $p - 1$.*

Proof. The pseudo-solution g of the system (3) is a solution of the square system

$$A^*Ag = \begin{pmatrix} f \\ O \end{pmatrix}. \tag{8}$$

The matrix of the system has the form

$$A^*A = \begin{bmatrix} I_{n_1} & O \\ O & O \end{bmatrix} + D_p^* D_p.$$

Let $\delta = D_p g$ be the vector consisting of the finite differences of the solution. We split it into two subvectors, δ_1 and δ_2, consisting of $n_1 - p$ and n_2 components, respectively. Then, the n_2 bottom rows of the system (8) are equivalent to the equality

$$R_{n_2}^* \delta_2 = 0,$$

where the matrix R_{n_2} is defined above (5). Since the matrix R_{n_2} is nonsingular, then $\delta_2 = 0$. This means that the finite differences of order p for the solution components $g_{n_1+1}, \ldots, g_{n_2}$ corresponding to the extrapolation interval are equal to zero. It follows that the extrapolation is a polynomial function of order $p - 1$. □

4 Numerical experiments

Experiment 1. In this experiment, we define a uniform grid on the interval $[\pi - 2, \pi + 2]$ with a step $h \in \{0.1,\ 0.05,\ 0.025,\ 0.0125\}$. On the subinterval $[\pi - 2, \pi]$ (the interpolation interval), the functions $\sin(x)$ and $\cos(x)$ are defined, and on the subinterval $(\pi, \pi + 2]$, extrapolation is performed. The results are shown in Fig. 1, 2. Let us pay attention to the error graphs. On the interval $[\pi - 2, \pi]$, the graphs actually show the approximation error. As can be seen, it is quite low and generally depends on the grid step h and the order p. On the extrapolation interval, the errors exhibit non-monotonic behavior. If the parity of the degree of the extrapolating polynomial does not coincide with the parity of the given function (even $p - 1$ for $\sin(x)$ and odd for $\cos(x)$), near the boundary $x = \pi$, the graphs corresponding to smaller values of h are lower than the others, but with distance from this point, the graphs intersect. This means that the error for large h becomes smaller than for small ones. Obviously, this phenomenon is related to the parity of the expansion of the function in a power series, but its mechanism is unclear.

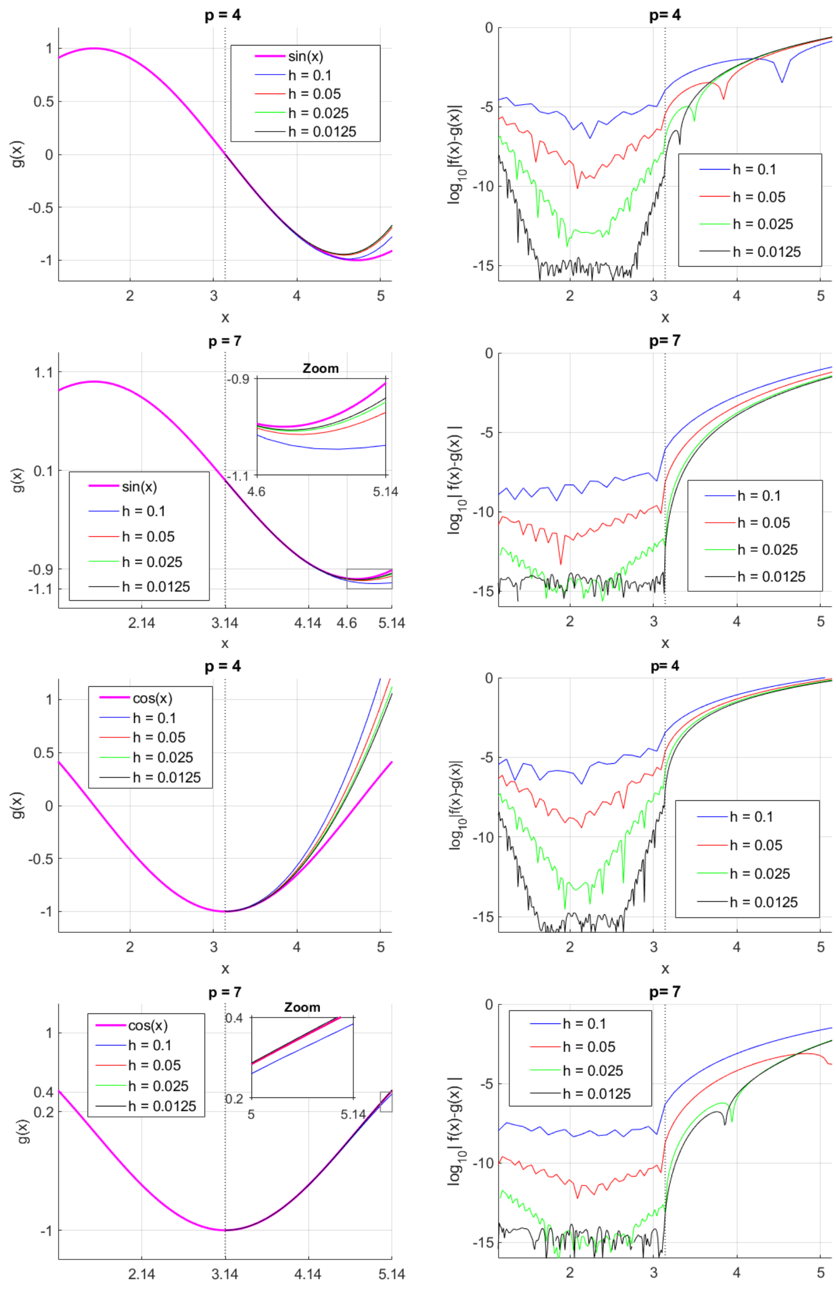

FIG. 1. Comparison of the functions $\sin(x)$, $\cos(x)$ and the obtained extrapolation with different steps h (left), error graphs (right).

Experiment 2. This section presents examples of calculations for a rapidly growing function $\exp(x)$ and for a function $\tan(x)$ with vertical asymptotics.

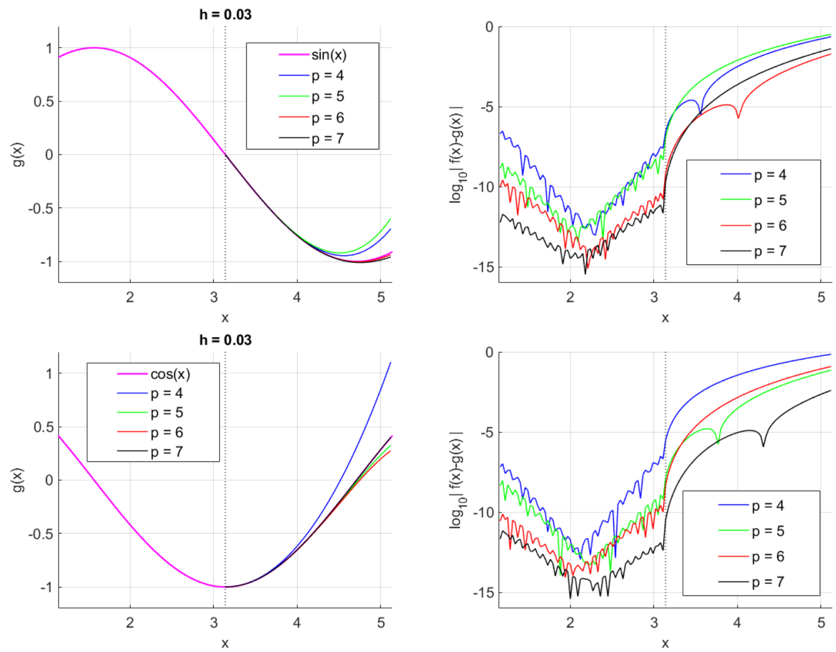

FIG. 2. Comparison of the functions $\sin(x)$, $\cos(x)$ and the obtained extrapolation for different values of p.

For the exponential, the interpolation and extrapolation intervals are the same as in the previous example. For the tangent, these are $[0,\ pi/4]$ and $(\pi/4, \pi/2]$, respectively. As expected, the growth of the function affects the accuracy of the extrapolation. With increasing distance from the interpolation interval, the error graphs for all considered values of h increase and converge together (Fig. 3). If h is fixed and the order of the finite differences p increases, the error level decreases significantly (Fig. 4).

Experiment 3. This section presents the results of numerical experiments for nonsmooth functions. Let us consider the function $f(x) = x\log_{10}|x|$, which at zero we complement with a zero value by continuity. Let us fix the interpolation $[-0.2, 0.4]$ and extrapolation $(0.4, 1]$ intervals. Fig. 5 shows a comparison of extrapolation continuations for several values of the grid step h and orders p. Of greatest interest is the dependence of extrapolation on p. As can be seen, the sequence of extrapolations diverges as their smoothness increases.

A similar situation occurs with the extrapolation of the function $|x|$. Although for a fixed p the accuracy increases with decreasing grid step, for a fixed step, divergence is observed with increasing p (Fig. 5). Therefore, to improve the extrapolation accuracy by increasing the order of p, sufficient smoothness of the given function is required.

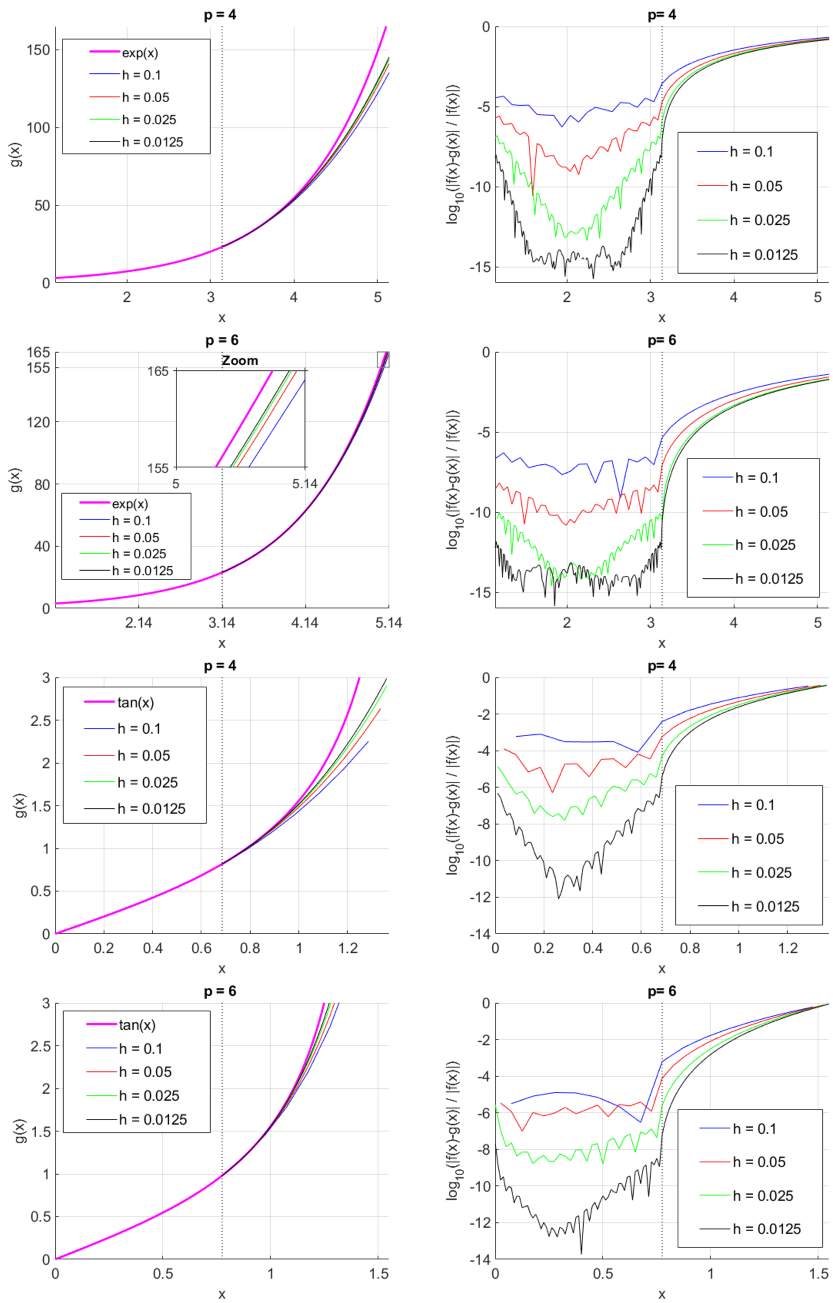

FIG. 3. Comparison of the functions $\exp(x)$, $\tan(x)$ and the obtained extrapolation with different steps h (left), graphs of the relative error $\log_{10}|(f(x)-g(x))/f(x)|$ (right).

Experiment 4. Let's compare the proposed method with the classical extrapolation method. To do this, we construct an interpolation polynomial

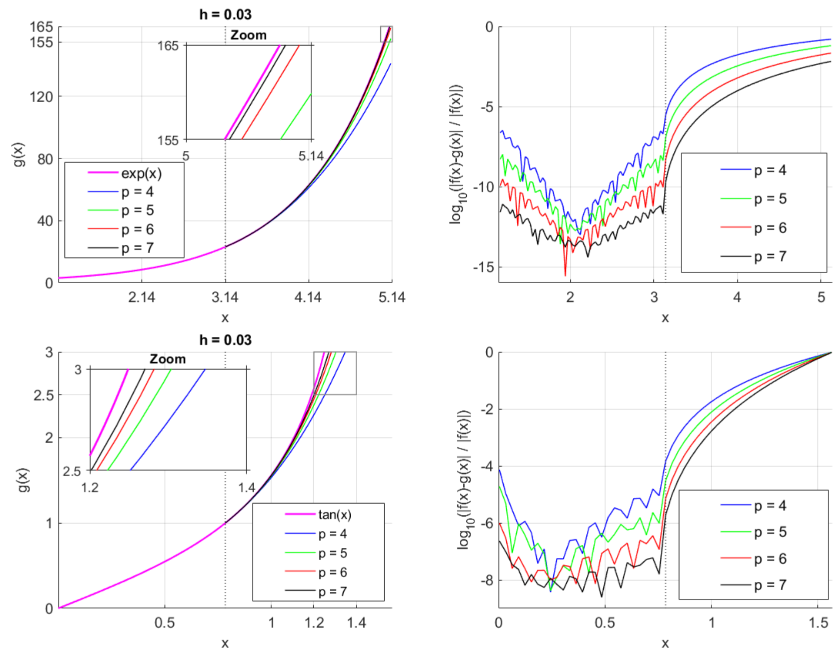

FIG. 4. Comparison of the functions $\exp(x)$, $\tan(x)$ and the obtained extrapolation for different p.

of degree m on the interpolation portion of the interval for the given values and extend it to the extrapolation region. There, we compare its values with the given function, as well as with the extrapolation using finite differences of different orders p and for different h. Note that, by Theorem 2, for $m = p-1$, both extrapolations are polynomials of the same degree m.

In Fig. 6, 7, this comparison is performed for the functions $\sin(x)$, $\cos(x)$, $\exp(x)$. The results obtained allow us to make the following observation: when comparing polynomial extrapolations of equal degrees, i.e., for $m = p - 1$, the extrapolation obtained by the new method yields a better approximation of the given function. When comparing the results of extrapolations for $m = p$, the result is variable and depends on the given function and the step h. The better approximation for equal degrees is likely due to more complete use of information about the given function in the interpolation interval.

Conclusion.

Thus, using the concept of Godunov regularization allowed us to develop a new, original numerical method for extrapolating functions defined on a grid. The method is based on solving a regularized linear system of algebraic equations. An estimate was obtained for the condition number of this system, which depends on the number of grid points and on p. This estimate allows

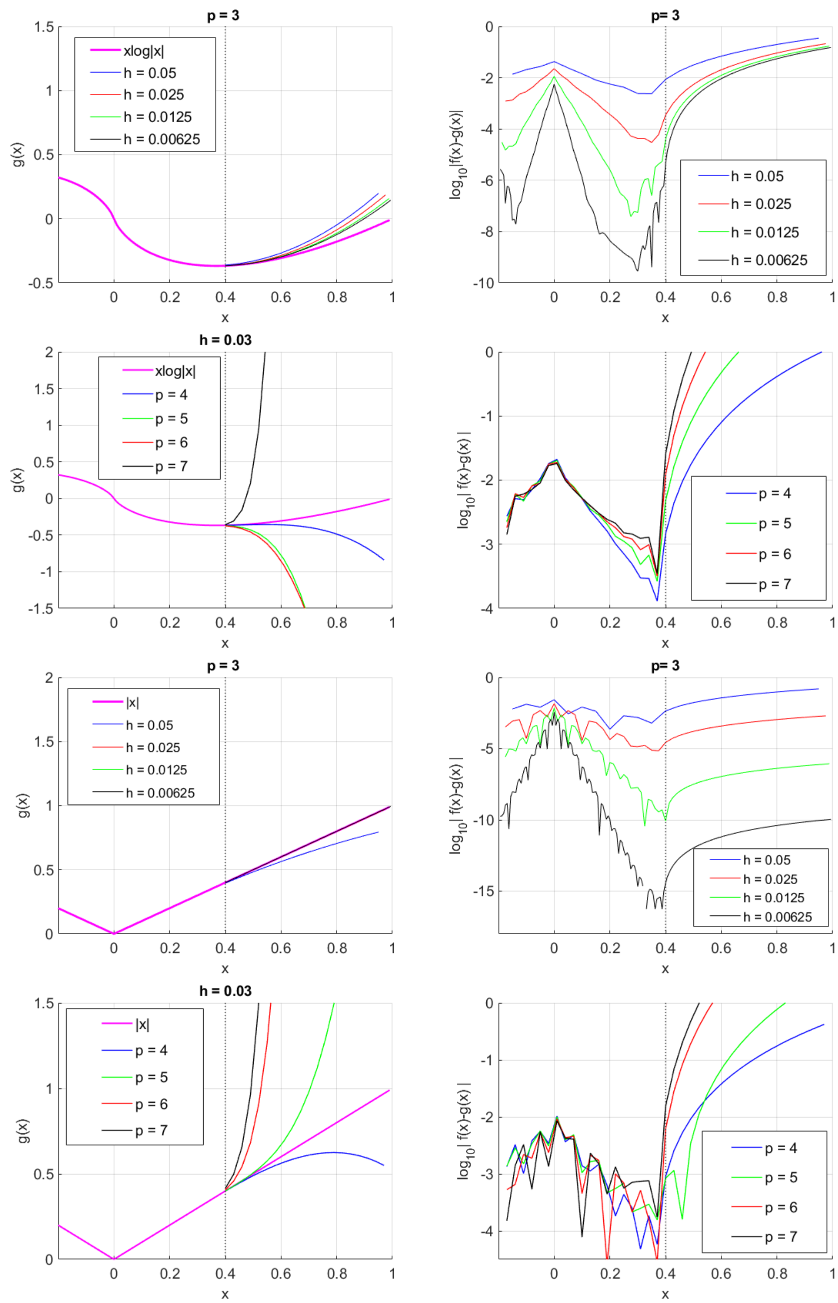

FIG. 5. Comparison of the functions $x \log |x|$, $|x|$ and the obtained extrapolation (left), error graphs (right), with different steps h at the top, with different order p at the bottom.

us to select the method parameters so that the computational error in solving the linear system does not significantly affect the final result.

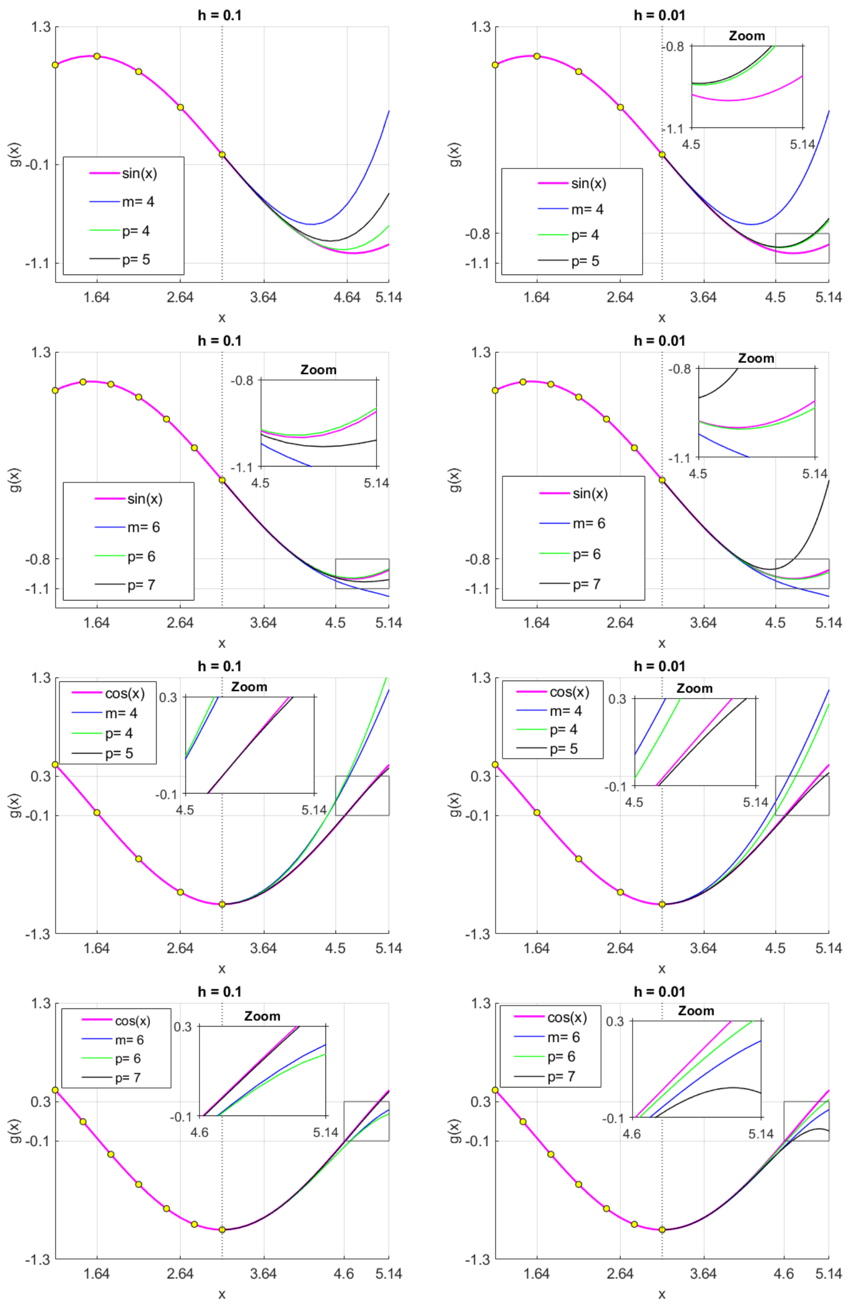

FIG. 6. Comparison of the results of extrapolation of the functions $\sin x$ and $\cos x$ using interpolation polynomials of degree m and using a new method using finite differences of order p on a grid with step h.

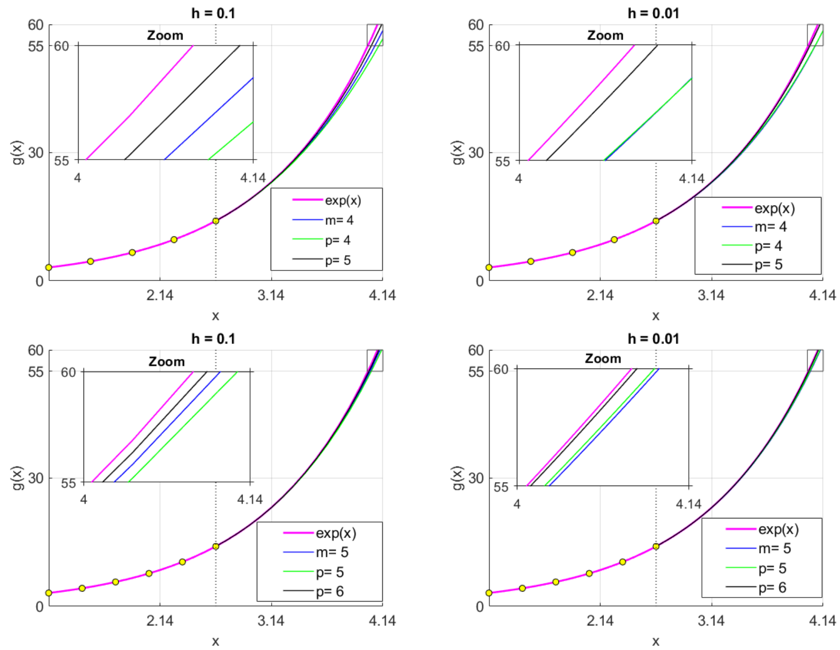

FIG. 7. Comparison of the results of extrapolation of the function $\exp x$ using interpolation polynomials of degree m and using a new method using finite differences of order p on a grid with step h.

It has been established that on the extrapolation interval the approximate function constructed in this way is a polynomial.

Several properties of the new extrapolation are illustrated with examples. It is noted that for sufficiently smooth functions, the extrapolation sequences converge both as the grid step h decreases and as the order of the finite differences p increases. However, if the function is extrapolated without regard to its parity, the error dependence on h is non-monotonic. In some cases, the extrapolation values are more accurate when using a coarser grid. The patterns of this behavior are not fully understood and require further study. If the given function is not smooth over the interval interval, then the extrapolation sequence diverges with increasing p. Furthermore, in numerical experiments, the extrapolation obtained by the proposed method proved to be more accurate than extrapolation using an interpolation polynomial of the same degree.

The obtained results allow us to assume that this method can be successfully applied in extrapolation problems in the presence of a priori information about the smoothness of the function.

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Elina Arnoldovna Biberdorf
Sobolev Institute of Mathematics,
pr. Koptyuga, 4,
630090, Novosibirsk, Russia
Email address: elina@biberdorf.ru

Kuvondik Kakhramanovich Abdisheripov
Novosibirsk State University,
ul. Pirogova, 1
630090, Novosibirsk, Russia
Email address: k.abdisheripov@g.nsu.ru