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Fast and correct computation of spectral representations of functions on Chebyshev grids

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Abstract. The Chebyshev collocation method (CCM) has been successfully and actively used for many years in the numerical solution of differential and integral equations, primarily linear ones. The purpose of this paper is to demonstrate the particularly convenient algebraic structure of the Chebyshev collocation method, which is clearly evident when applied to function interpolation. This article explores several different approaches to using special interpolation grids and the properties of discrete orthogonality with respect to differently preconditioned Chebyshev matrices whose Gram matrix is diagonal. Each of the proposed methods enables the robust calculation of the coefficients of the expansion in Chebyshev polynomials of both the first and second kind for the functions under study. In essence, multiplying the transposed matrix by the vector of function values at grid points yields the coefficients of the expansion of this function in Chebyshev polynomials. Using the Clenshaw method reduces the complexity of this operation to that of the discrete cosine transform (Fourier) for an arbitrary number of interpolation points. Using this approach allows us to dramatically simplify calculations when solving differential and integral equations.

Obtaining the coefficients of the derivative expansion is reduced to multiplying the vector of interpolation coefficients by an upper-triangular differentiation matrix. The coefficients of the antiderivative are obtained by simply multiplying the bidiagonal integration matrix by the vector of interpolation coefficients of the function. Thus, the Chebyshev interpolation method demonstrates the highest efficiency of the collocation method.

Keywords: Interpolation, Chebyshev Polynomials, Collocation Methods, Grids of First and Second Kind

MSC numbers: 83C55, 83C57

1. Introduction

Ordinary differential equations are effective tools for modeling various natural processes and technical systems. The polynomial collocation method, a powerful numerical approach, serves as a reliable method for efficiently solving both differential and integro-differential equations. This article discusses the application of the collocation method to calculating the expansion coefficients of an interpolated function, such as the solution to a differential equation, in a series in a system of Chebyshev polynomials of the first and second kind.

Since its inception in the 20th century [1, 2] (see [19]), the collocation method has been widely used to solve differential and integro-differential equations. The method's effectiveness stems from its ability to reduce the solution of differential equations to the solution of algebraic linear or nonlinear systems. This approach, through the selection of special interpolation grids, allows for the solution of linear algebraic equations (SLAEs) with completely populated matrices.

The basis of spectral collocation methods for solving ODEs is the approximation of the desired function by an interpolation polynomial, which is its expansion in a series in basis functions. Finite sums of global basis functions are used [21], which must satisfy the differential equation at specific collocation points-nodes. Chebyshev basis functions, together with the choice of specialized non-uniform grids (for which the coordinates of the collocation points are known in analytical form [27]), make it possible to simplify the computational complexity of finding the interpolation coefficients and ensure a “spectral” (exponential) rate of convergence [4].

Function approximation has been a central topic in numerical analysis since its inception. One of the most efficient methods for approximating a function $f : [-1, 1] \to \mathbb{R}$ is to use an interpolation polynomial P_N of degree P_N satisfying the collocation condition $P_N(x_j) = F(x_j)$ for the set of $(N+1)$ interpolation points $\{x_j\}, j = 0, 1, \ldots, N$. In practice, the Chebyshev points of the second kind $x_k = \cos\left(\frac{k\pi}{n}\right)$, $k = 0, \ldots, n$ are usually chosen as the interpolation points. In this case, the resulting interpolation polynomial, known as the Chebyshev interpolant, serves as a near-optimal approximation of the function $f(x)$ in the space of polynomials of degree at most $(N + 1)$ [6]. A common basis for representing the interpolation polynomial P_N is also a basis of Lagrange polynomials, and the calculation of P_N in this basis can be stably performed using the barycentric interpolation formula [4, 7].

Other often used bases include Newton polynomials, Chebyshev polynomials of the second kind, and Legendre polynomials. Alternatively, to represent P_N, one can use (the most obvious one) a monomial basis such that $P_N(x) = \sum_{k=0}^{N} a_k x^k$ for the coefficients $\{a_k\}$. Computing the coefficient vector of monomials $a^{(N)} := (a_0, a_1, \ldots, a_N)^T \in \mathbb{R}^{(N+1)}$ of the interpolating polynomial P_N requires solving the linear system $V^{(N)}a^{(N)} = f^{(N)}$, where

$$V^{(N)} = \begin{pmatrix} 1 & x_0 & x_0^2 & \cdots & x_0^N \\ 1 & x_1 & x_1^2 & \cdots & x_1^N \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_N & x_N^2 & \cdots & x_N^N \end{pmatrix} \in \mathbb{R}^{(N+1)\times(N+1)}$$

is the Vandermonde matrix, $f^{(N)} = (F(x_0), F(x_1), \ldots, F(x_N))^T \in \mathbb{R}^{(N+1)}$ is the vector of values of the function F at $(N+1)$ interpolation points on the interval $[-1, 1]$.

It is well known that for any set of real interpolation points [24] within the unit interval, the condition number $V(N)$ grows at least as fast as $\dfrac{\sqrt{2}(1+\sqrt{2})^{N-1}}{\sqrt{N+1}}$ [8]. It follows that the accuracy of the numerical solution of this linear system rapidly deteriorates with increasing N, and, therefore, this algorithm for constructing P_N is considered unstable [24].

The polynomial collocation (interpolation) method has proven itself in solving problems such as:

- integrating first- and second-order LODEs [9, 10, 11];
- calculating definite integrals of rapidly oscillating functions[1][13, 14].

In both cases, the computational core of the solution is the restoration of the interpolating polynomial (interpolant) of degree $\leq n$ in the space of polynomials $\dim = n + 1$ using $(n + 1)$ collocation points $\{x_0, x_1, \ldots, x_n\}$.

In Refs. [10, 11, 13, 14], Chebyshev polynomials of the first kind were mainly used, and the sets of Chebyshev–Lobatto points (extrema of the polynomial T_{n+1}, the points of the second kind) [15, 16] were chosen as collocation points, as they are more common in the interpolation of the desired functions.

In order for polynomial interpolation to be a well-conditioned process, it is necessary to abandon uniformly distributed points [4, 17, 24]. As is well known in approximation theory, the correct approach is to use sets of points grouped at the ends of the interval [29] with an asymptotic density proportional to $(1-x^2)^{-1/2}$ as $n \to \infty$ in the case of T_{n+1} and $(1-x^2)^{1/2}$ in the case of $(1-x^2)U_n$ [4]. The simplest examples of cluster sets of points are the Chebyshev point families [29], obtained by projecting uniformly spaced points on the upper semicircle onto the interval $[-1, 1]$. Four standard varieties of such points are known for polynomials

[1] As a benchmark calculation for the Chebyshev polynomial bases, one can point to the problem of finding the spectrum of a hydrogen atom on a three-dimensional sphere, proposed in the work [12]. In this paper the radial Schrodinger equation for the wave functions in discrete the momentum representation for central potentials on a three-dimensional sphere are obtained in the form of a system of homogeneous algebraic equations. The numerical method of calculation of quasiradial solutions and spectrum is proposed on the basis of the Chebychev procedure of constructing a suitable system of orthogonal polynomials of a discrete variable.

of the 1st, 2nd, 3rd, and 4th kind, and for each of them there is an explicit formula for calculating the points of a special interpolation grid [18].

A minor modification of the SLAE matrix of the collocation method allows [25] to achieve diagonalization [25] of the Gram matrix by selecting collocation points and using the discrete orthogonality of Chebyshev polynomials. Thus, the algorithm for finding the interpolant expansion coefficients is reduced to multiplying the matrix, transposed with respect to the collocation method matrix, by the vector of values of the approximated function at the collocation points. An even greater acceleration of calculations can be achieved by using the Clenshaw algorithm for multiplying the Chebyshev matrix by a vector and using the symmetry of the location of the collocation points relative to the origin.

Similar advantages (the analytical form of the “almost” inverse matrix) can be obtained by searching for an interpolant, i.e., expanding the interpolated function in Chebyshev polynomials of the first kind and choosing the Chebyshev–Gauss grid (points of the first kind) as the collocation points. Modified Chebyshev polynomials of the second kind, having the form $(1-x^2)U_n$, can also be used as basis functions to create equally efficient and robust algorithms for interpolating functions and solving ODEs and integral equations. The use of discrete “orthogonality” (diagonalization of the corresponding Gram matrix) is best shown by choosing the zeros or extrema of modified Chebyshev polynomials of the second kind as the collocation points.

To consider specific options for formulating the interpolation problem based on the collocation method, we present some preliminary information.

2. Theoretical foundations of the method

To solve differential equations numerically, spectral methods are used [21, 5], based on the representation of the function under study in the form of a finite series

$$u_n(x) = \sum_{j=0}^{n} c_j \varphi_j(x),$$

where Chebyshev polynomials of the first and second kinds are considered as the basis functions $\varphi_j(x)$ in the solution described in this paper. Let us examine the properties of Chebyshev polynomials in more detail to justify this choice.

Chebyshev polynomials of the first and second kinds stand for two sequences of orthogonal polynomials related to the cosine and sine functions, denoted as $T_n(x)$ and $U_n(x)$, respectively. They can be defined in several equivalent ways; below, we will define them using trigonometric functions:

Chebyshev polynomials of the first kind T_n [20] are defined by the formula

$$T_n(\cos\theta) = \cos(n\theta),$$

and Chebyshev polynomials of the second kind U_n are defined by the formula

$$U_n(\cos\theta)\sin\theta = \sin((n+1)\theta).$$

2.1 Chebyshev polynomials of the first kind

Chebyshev polynomials of the first kind $T_n(x)$ defined on the segment $[-1, 1]$ can be explicitly expressed as

$$T_n(x) = \cos(n \arccos x),$$

they satisfy the following recursion relation [20]

$$T_{n+1}(x) = 2xT_n(x) - T_{n-1}(x),$$

with initial conditions

$$T_0(x) = 1, \quad T_1(x) = x.$$

This method of definition allows significant simplification when calculating the values of basis functions. Due to the recurrent structure, the complexity of calculating the values of all basis functions up to order n is linear in n.

Polynomials $T_n(x)$ form an orthogonal system in the space $L^2([-1, 1], w(x))$ with weight

$$w(x) = \frac{1}{\sqrt{1 - x^2}},$$

i.e., the orthogonality condition holds [20]

$$\int_{-1}^{1} T_m(x)T_n(x)\frac{dx}{\sqrt{1-x^2}} = \begin{cases} 0, & m \neq n, \\ \pi, & n = 0, \\ \dfrac{\pi}{2}, & n \geq 1. \end{cases}$$

Continuous orthogonality underlies the emergence of discrete orthogonality on special Chebyshev grids, which are further used in the collocation method.

2.2 Chebyshev polynomials of the second kind

Chebyshev polynomials of the second kind $U_n(x)$ are defined by the formula [20]

$$U_n(x) = \frac{\sin((n + 1) \arccos x)}{\sin(\arccos x)},$$

and satisfy the recurrence relation

$$U_{n+1}(x) = 2xU_n(x) - U_{n-1}(x),$$

and initial conditions

$$U_0(x) = 1, \quad U_1(x) = 2x.$$

As for polynomials of the first kind, a similar recurrence formula ensures linear computational complexity when calculating the values of the interpolant.

The polynomials $U_n(x)$ form an orthogonal system in the space $L^2([-1, 1], \tilde{w}(x))$ with the weight

$$\tilde{w}(x) = \sqrt{1 - x^2},$$

i.e., the following relation holds:

$$\int_{-1}^{1} U_m(x)U_n(x)\sqrt{1-x^2}\,dx = \begin{cases} 0, & m \neq n, \\ \frac{\pi}{2}, & m = n. \end{cases}$$

Unlike polynomials of the first kind, the weight function of polynomials of the second kind vanishes at the boundaries of the interval, therefore, to bring the matrix of the system to diagonal form, it is necessary to take into account the weights when solving, however, for Chebyshev polynomials of the second kind on a grid of the second kind, the boundary values vanish due to the weights, which is important to be taken into account in the future.

2.3 Collocation method for solving interpolation problems

The primary method for working with Chebyshev polynomials when solving numerical problems is the collocation method [23], since this method utilizes the discrete orthogonality of polynomials, and the solution is reduced to multiplying a diagonal matrix by a vector. Let's examine this method in more detail.

Let the function $f(x)$ be defined at nodes x_k. The interpolation polynomial is represented as a finite sum

$$u_n(x) = \sum_{j=0}^{n} c_j \phi_j(x),$$

where $\phi_j(x)$ are the basis functions (Chebyshev polynomials of the proper kind).

The determination of the expansion coefficients c_j is reduced to solving a system of linear algebraic equations found by the collocation conditions

$$u_n(x_k) = f(x_k).$$

In matrix form the system is written as

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

where $A_{kj} = \phi_j(x_k)$.

The system of equations (1) has a unique solution when searching for the expansion of a function in a series of Chebyshev polynomials (of the first and second kind) in the absence of coinciding grid nodes $x_k,\ k = 0, \dots, n$.

For an arbitrary grid of nodes, the matrix of such a system of equations will be completely filled, and the complexity of finding the expansion coefficients is $O(n^3)$. However, a special choice of collocation nodes, as mentioned earlier, allows one to use the discrete orthogonality of Chebyshev polynomials or their modifications to calculate the desired coefficients due to the diagonal structure of the corresponding Gram matrix

$$G = A^T A.$$

Thus, practically the solution of the general system of linear equations (1) is reduced to multiplying the transposed matrix A^T of the equation by the vector of function values $f(x_k)$, $k = 0, \ldots, n$. Advantages and simplicity of this approach to finding the interpolant expansion coefficients are obvious.

2.4 Chebyshev nodes and discrete orthogonality

In numerical analysis, Chebyshev nodes (also called Chebyshev points or Chebyshev meshes) are a set of specific algebraic numbers used as nodes for polynomial interpolation and numerical integration. They are the projection of a set of evenly spaced points on the unit circle onto the real interval $[-1, 1]$, i.e., onto the diameter of the unit circle.

There are two kinds of Chebyshev nodes [16, 23, 26]. n Chebyshev nodes of the first kind, also called Chebyshev–Gauss nodes[1], are zeros of Chebyshev polynomial of the first kind, $T_n(x)$ (see fig. 1). The corresponding $(n+1)$ Chebyshev nodes of the second kind also called Chebyshev–Lobatto nodes[2], are extrema of the polynomial $T_n(x)$. These nodes are also zeros of Chebyshev polynomial of the second kind $U_{n-1}(x)$ together with the added ends of the interval $[-1, 1]$ (see fig. 2). Both types of numbers are commonly called Chebyshev nodes [27] or Chebyshev points in the literature.

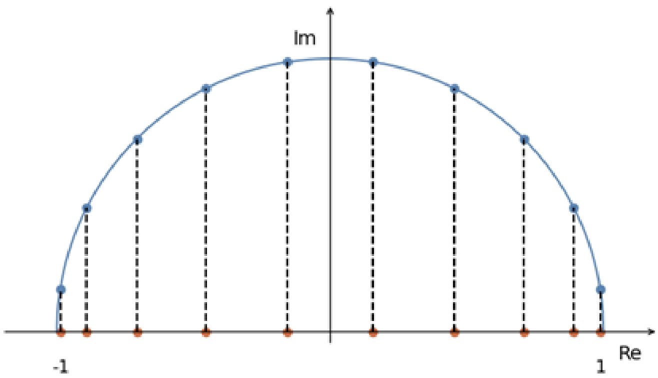

Figure 1: Constructing a grid of points of the first kind

The aim of this paper is to present an economical, robust method for calculating the spectral coefficients of the expansion of an interpolated function into a series of Chebyshev polynomials of the first and second kind. Specific examples are considered below.

[1]The name “Chebyshev–Gauss nodes” comes from the use of Chebyshev zeros in numerical integration, which can be thought of as a variant of Gaussian quadrature.

[2]The name “Chebyshev–Lobatto nodes” comes from the name of R. Lobatto, who created a version of Gauss quadrature, known as Lobatto quadrature, whose nodes included the endpoints of the interval – a feature inherent in the extrema of Chebyshev polynomials.

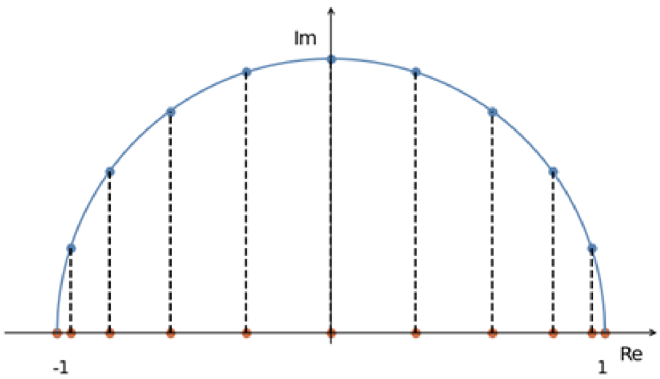

Figure 2: Constructing a grid of points of the second kind

Chebyshev polynomials of the first kind. Chebyshev nodes of the first kind.

Chebyshev nodes of the first kind are expressed as [23, 26]

$$x_k = \cos\left(\frac{(k+1/2)\pi}{n}\right), \quad k = 0, \dots, n-1.$$

These nodes do not include boundary points of the interval and are found strictly inside. The elements of the collocation matrix have the form

$$A_{kj} = T_j(x_k) = \cos\left(j\frac{(k+1/2)\pi}{n}\right).$$

In this case, the Gram matrix also turns out to be diagonal due to the discrete orthogonality of the cosine system.

Diagonal structure of the Gram matrix

Theorem 1. *The Gram matrix of the collocation method when expanding the interpolated function into a series of Chebyshev polynomials of the first kind on a grid of the first kind has the form*

$$G = A^T A = \begin{pmatrix} n & 0 & 0 & \cdots & 0 \\ 0 & \frac{n}{2} & 0 & \cdots & 0 \\ 0 & 0 & \frac{n}{2} & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & \frac{n}{2} \end{pmatrix}$$

Proof.

Let us consider the values of the elements of the Chebyshev interpolation matrix on a grid of nodes of the first kind. Let θ_k be expressed as

$$\theta_k = \frac{(k+1/2)\pi}{n}.$$

Then

$$A_{kj} = \cos(j\theta_k)$$

The Gram matrix has elements

$$G_{ij} = \sum_{k=0}^{n-1} \cos(i\theta_k)\cos(j\theta_k).$$

Using the cosine product formula

$$cos(i\theta)\cos(j\theta) = \frac{1}{2}[\cos((i-j)\theta) + \cos((i+j)\theta)],$$

we get

$$G_{ij} = \frac{1}{2}\sum_{k=0}^{n-1}\cos((i-j)\theta_k) + \frac{1}{2}\sum_{k=0}^{n-1}\cos((i+j)\theta_k).$$

From the properties of discrete trigonometric sums, it follows that

$$\sum_{k=0}^{n-1}\cos(m\theta_k) = \begin{cases} n, & m = 0, \\ 0, & m \neq 0. \end{cases}$$

Therefore,

$$G_{ij} = \begin{cases} n, & i = j = 0, \\ \frac{n}{2}, & i = j \neq 0, \\ 0, & i \neq j. \end{cases}$$

Thus, the Gram matrix is diagonal. There is no case $i = j = n$, since $x_k = \cos\left(\frac{(k+1/2)\pi}{n}\right)$, $k = 0, \ldots, n-1$.

Then the coefficients for the Chebyshev polynomials of the first kind for the grid of the first kind will be calculated in an analogous way

$$c_k = (G^{-1})_{kk}\tilde{f}_k, \quad k = 0, \ldots, n.$$

Chebyshev polynomials of the first kind. Chebyshev nodes of the second kind

The Chebyshev nodes of the second kind are calculated using the explicit formula [23]

$$x_k = \cos\left(\frac{k\pi}{n}\right), \quad k = 0, \ldots, n.$$

This set of nodes includes the boundary points of the interval $[-1,1]$. When using these nodes, the values of basis functions at the grid points are expressed as

$$T_j(x_k) = \cos\left(j\frac{k\pi}{n}\right), \quad k = 0,\dots,n;\ j = 0,\dots,n.$$

The matrix of the system of equations of the collocation method $Ac = f$ for calculating the coefficients of the expansion of a certain function in a series of Chebyshev polynomials of the first kind has the form

$$\begin{pmatrix} T_0(x_0) & T_1(x_0) & T_2(x_0) & \cdots & T_n(x_0) \\ T_0(x_1) & T_1(x_1) & T_2(x_1) & \cdots & T_n(x_1) \\ T_0(x_2) & T_1(x_2) & T_2(x_2) & \cdots & T_n(x_2) \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ T_0(x_n) & T_1(x_n) & T_2(x_n) & \cdots & T_n(x_n) \end{pmatrix} \begin{pmatrix} c_0 \\ c_1 \\ c_2 \\ \vdots \\ c_n \end{pmatrix} = \begin{pmatrix} f_0 \\ f_1 \\ f_2 \\ \vdots \\ f_n \end{pmatrix}$$

To obtain discrete orthogonality at the boundary points, the collocation matrix is modified [25], which consists of multiplying the first and last rows by a factor of $\frac{1}{\sqrt{2}}$, then the modified system on the left is multiplied by the transposed matrix. As a result, the corresponding Gram matrix

$$G = A^T A = \begin{pmatrix} n & 0 & 0 & \cdots & 0 \\ 0 & \frac{n}{2} & 0 & \cdots & 0 \\ 0 & 0 & \frac{n}{2} & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & n \end{pmatrix}$$

acquires a diagonal structure, which allows one to calculate the expansion coefficients without solving the full system of linear equations, but only by multiplying the matrix G by the transformed vector of values of the interpolated function $\tilde{f} = \left(\frac{f_0}{\sqrt{2}}, f_1, \dots, f_{n-1}, \frac{f_n}{\sqrt{2}}\right)^T$, $k = 0,\dots,n$.

$$\begin{pmatrix} n & 0 & 0 & \cdots & 0 \\ 0 & \frac{n}{2} & 0 & \cdots & 0 \\ 0 & 0 & \frac{n}{2} & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & n \end{pmatrix} \begin{pmatrix} c_0 \\ c_1 \\ c_2 \\ \vdots \\ c_n \end{pmatrix} = \begin{pmatrix} \tilde{f}_0 \\ \tilde{f}_1 \\ \tilde{f}_2 \\ \vdots \\ \tilde{f}_n \end{pmatrix}$$

Thus, the expansion coefficients are found by the formula

$$c_k = \tilde{f}_k / G_{kk}, \quad k = 0,\dots,n.$$

Chebyshev polynomials of the second kind. The grid of nodes of the first kind

The nodes of the second kind are given by the expression

$$x_k = \cos\left(\frac{k\pi}{n+1}\right), \quad k = 1, \ldots, n.$$

The collocation matrix elements are calculated using the formula

$$A_{kj} = U_j(x_k).$$

In this case, the Gram matrix also turns out to be diagonal because of discrete orthogonality of the sine system:

$$G = A^T A = \begin{pmatrix} \frac{n}{2} & 0 & 0 & \cdots & 0 \\ 0 & \frac{n}{2} & 0 & \cdots & 0 \\ 0 & 0 & \frac{n}{2} & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & \frac{n}{2} \end{pmatrix}$$

Derivation of the Gram matrix diagonal structure

Theorem 2. *The Gram matrix of the collocation method when expanding the interpolated function into a series of Chebyshev polynomials of the second kind on a grid of nodes of the first kind has a diagonal form*

$$G = A^T A = \begin{pmatrix} \frac{n+1}{2} & 0 & \cdots & 0 \\ 0 & \frac{n+1}{2} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \frac{n+1}{2} \end{pmatrix}$$

Proof.
Consider the values of the collocation matrix elements

$$A_{kj} = U_j(x_k),$$

where the grid nodes are given by the expression

$$x_k = \cos\left(\frac{k\pi}{n+1}\right), \; k = 1, \ldots, n.$$

Using the trigonometric representation of Chebyshev polynomials of the second kind

$$U_j(\cos\theta) = \frac{\sin((j+1)\theta)}{\sin\theta},$$

we obtain

$$U_j(x_k) = \frac{\sin((j+1)\theta_k)}{\sin\theta_k}$$

at $\theta_k = \frac{k\pi}{n+1}$ and $w_k = \sin^2\left(\frac{k\pi}{n+1}\right)$.

As a result of multiplying $U_j(x_k)$ by all w_k we get

$$\tilde{A}_{kj} = \sin((j+1)\theta_k).$$

The Gram matrix elements have the form

$$G_{ij} = \sum_{k=1}^{n} \sin((i+1)\theta_k)\sin((j+1)\theta_k).$$

Using the formula for a product of sines

$$\sin a \sin b = \frac{1}{2}[\cos(a-b) - \cos(a+b)],$$

we get

$$G_{ij} = \frac{1}{2}\sum_{k=1}^{n}\cos((i-j)\theta_k) - \frac{1}{2}\sum_{k=1}^{n}\cos((i+j+2)\theta_k).$$

From the properties of discrete trigonometric sums, it follows that

$$\sum_{k=1}^{n}\cos(m\theta_k) = \begin{cases} n+1, & m=0, \\ 0, & m\neq 0. \end{cases}$$

Therefore

$$G_{ij} = \begin{cases} \dfrac{n+1}{2}, & i=j, \\ 0, & i\neq j. \end{cases}$$

Thus, the Gram matrix is diagonal. Then the expansion coefficients are found by the formula

$$c_k = (G^{-1})_{kk}\tilde{f}_k, \quad k = 0,\ldots,n.$$

Expansion in Chebyshev polynomials of the second kind. The nodes of the second kind

The nodes of the second kind are determined by the formula [23, 21]

$$x_k = \cos\left(\frac{k\pi}{n}\right), \quad k = 0,\ldots,n.$$

The collocation matrix elements have the form

$$A_{kj} = U_j(x_k).$$

The continuous orthogonality of the second-kind polynomials is fulfilled with the weight

$$w(x) = \sqrt{1-x^2}.$$

When moving to a discrete grid, weight arises

$$w_k = \sin^2\left(\frac{k\pi}{n}\right).$$

In this case

$$w_0 = 0,\ w_n = 0.$$

To take the weight into account, all elements of the matrix are multiplied by it

$$\tilde{A}_{kj} = \sqrt{w_k}\,U_j(x_k).$$

In the matrix form, the collocation systems are written as

$$\begin{pmatrix} \sqrt{w_1}U_0(x_1) & \sqrt{w_1}U_1(x_1) & \cdots & \sqrt{w_1}U_n(x_1) \\ \sqrt{w_2}U_0(x_2) & \sqrt{w_2}U_1(x_2) & \cdots & \sqrt{w_2}U_n(x_2) \\ \sqrt{w_3}U_0(x_3) & \sqrt{w_3}U_1(x_3) & \cdots & \sqrt{w_3}U_n(x_3) \\ \vdots & \vdots & \ddots & \vdots \\ \sqrt{w_{n-1}}U_0(x_{n-1}) & \sqrt{w_{n-1}}U_1(x_{n-1}) & \cdots & \sqrt{w_{n-1}}U_n(x_{n-1}) \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ \vdots \\ c_{n-1} \end{pmatrix} = \begin{pmatrix} f_1 \\ f_2 \\ f_3 \\ \vdots \\ f_{n-1} \end{pmatrix}$$

Since $w_0 = 0$, $w_n = 0$, the first and the last row of this matrix turn into zero. This means that the outermost nodes are formally present in the grid, but only the interior points are used in calculating the expansion coefficients.

The Gram matrix is defined by the expression

$$G = \tilde{A}^T\tilde{A} = \begin{pmatrix} \frac{n}{2} & 0 & & \cdots & 0 & 0 \\ 0 & \frac{n}{2} & & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \cdots & 0 & 0 \\ 0 & 0 & 0 & \frac{n}{2} & 0 & -\frac{n}{2} \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{n}{2} & 0 & \frac{n}{2} \end{pmatrix}$$

The diagonal structure of this matrix is obtained similarly to the derivation given earlier. However, the matrix is almost diagonal, since trigonometric functions are considered, and separation into real and imaginary parts occurs. As a result, when discretely calculating scalar products, some modes turn out to be pairwise coupled, which leads to the appearance of adjacent elements instead of a strictly single diagonal coefficient.

However, as can be seen in the image above, the matrix keeps a nearly diagonal structure, and we can still calculate the expansion coefficients without solving the full system of linear equations.

3 Accuracy assessment of numerical methods (Interpolation and differentiation error metrics)

In this paper, the interpolation residual [22, 28] is used to estimate the point, which is defined as

$$r_N(x) = f(x) - u_N(x).$$

The main characteristic of accuracy is the maximum residual norm [28]:

$$\|r_N\|_\infty = \max_{x\in[-1,1]} |r_N(x)|.$$

Calculation of $\|r_N\|_\infty$ is performed on a dense grid of $M = 400$ equally spaced points.

Additionally, the mean and root-mean-square errors at the collocation nodes are calculated:

$$\varepsilon_N = \frac{1}{K}\sum_{k=1}^{K} |f(x_k) - u_N(x_k)|, \qquad \varepsilon_N^{\text{RMS}} = \sqrt{\frac{1}{K}\sum_{k=1}^{K} |f(x_k) - u_N(x_k)|^2},$$

where K is the number of nodes ($K = N+1$ for Chebyshev polynomials of the first kind on a grid of the second kind, $K = N$ for the rest grids).

4. Analysis of convergence of spectral methods (exponential and algebraic convergence)

For smooth functions in the interval from -1 to 1 spectral methods using Chebyshev polynomials as basis functions show exponential convergence:

$$\|r_N\|_\infty \le C \cdot e^{-\alpha N}, \quad \alpha > 0,$$

where the constants C, α depend on the domain of analyticity of the function in the complex plane. In the program this dependence is studied by plotting $\log_{10}(\|r_N\|_\infty)$ versus N [22]: linear descent of the curve confirms exponential convergence.

In the presence of points of non-smoothness (discontinuities of derivatives), convergence becomes algebraic:

$$\|r_N\|_\infty \le C \cdot N^{-\beta}, \quad \beta > 0,$$

where the exponent β is found by the order of continuity of the function. The program for analyzing such behavior provides test functions with breaks, for example $f(x) = |x - a|$.

5. Practical part

5.1 Numerical examples at $n = 7$

An algorithm for constructing an interpolation based on Chebyshev polynomials was described above. A program for constructing a function interpolant was written using this algorithm. Smooth and nonsmooth functions were considered as test functions. We will give several examples to show the speed and accuracy of calculations using this method.

In all examples below, the grid parameter is set to $n = 7$.

Interpolation of the function $f_1(x) = \exp(\alpha(x^2 - 1))$ by Chebyshev polynomials of the first kind on a grid of nodes of the second kind

Consider the function

$$f_1(x) = \exp(\alpha(x^2 - 1)), \quad \alpha = 10.$$

Since the function changes rapidly near the endpoints of the interval, we will use Chebyshev polynomials of the first kind on a grid of nodes of the second kind, as they include the boundary points.

Using the algorithm described earlier, we find the original matrix using the formula $A_{kj} = T_j(x_k) = \cos(jk\pi/n)$ and multiply the first and last rows.

As a result of such transformations, the final Gram matrix $G = \tilde{A}^T \tilde{A}$ becomes diagonal:

$$G = \tilde{A}^T \tilde{A} = \begin{pmatrix} n & 0 & 0 & \cdots & 0 \\ 0 & \frac{n}{2} & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \cdots & 0 \\ 0 & 0 & 0 & \frac{n}{2} & 0 \\ 0 & 0 & 0 & 0 & n \end{pmatrix}$$

Therefore, the coefficients can be calculated using the formula

$$c_k = (G^{-1})_{kk} \tilde{f}_k,$$

where $\tilde{f}_k = \tilde{A}^T f_k$. With the obtained coefficients, we can directly construct the interpolant of the original function.

The resulting plot (fig. 3) shows that the interpolation polynomial reproduces the general shape of the original function, but there are noticeable deviations. This is because with a small number of nodes, the interpolation of the function does not provide sufficient accuracy, resulting in a residual value of $\max |r(x)| = 1.269 \times 10^{-1}$.

Moreover, the Gram matrix is diagonal, confirming the correct application of the spectral method and the orthogonality of the basis. Therefore, the main factor causing the error is not the method, but the insufficient number of nodes.

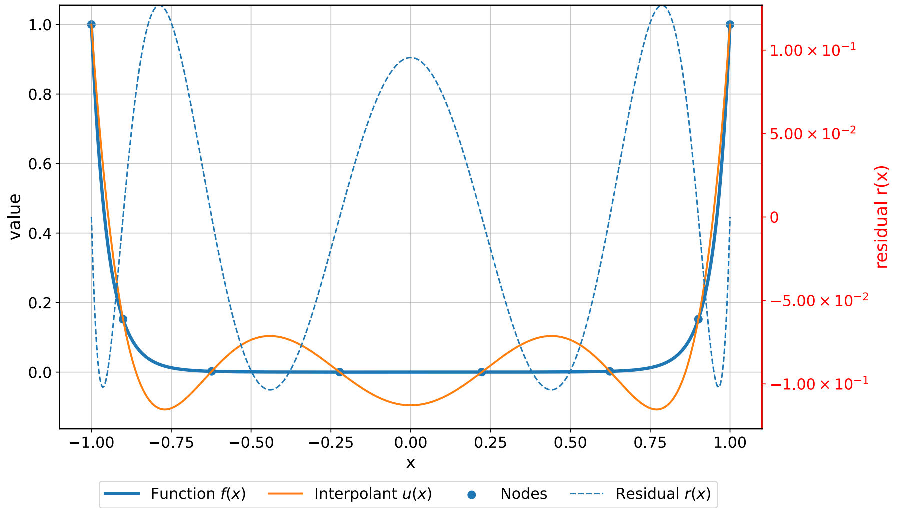

Figure 3: Interpolation of the function $f_1(x) = \exp\big(\alpha(x^2 - 1)\big)$ by Chebyshev polynomials of the first kind on a grid of 7 nodes of the second kind

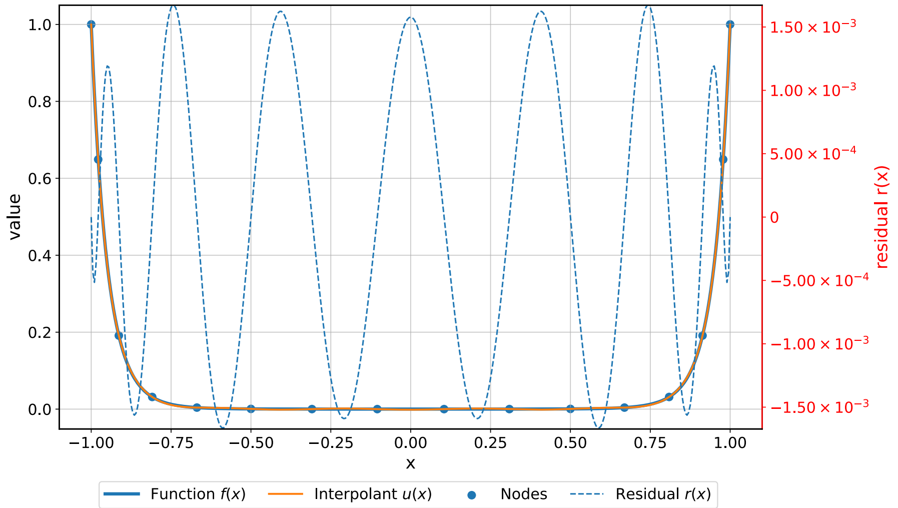

Figure 4: Interpolation of the function $f_1(x) = \exp\big(\alpha(x^2 - 1)\big)$ by Chebyshev polynomials of the first kind on a grid of 15 nodes of the second kind

To improve the interpolation accuracy, we increase the parameter and set $n = 15$.

With an increase in the number of nodes, a rapid decrease in the error is observed $\max|r(x)| = 1.672 \times 10^{-3}$, which corresponds to the exponential convergence of spectral methods for smooth functions, and the interpolant practically coincides with the function constructed analytically.

Interpolation of function $f_2(x) = \sin(\omega x)e^{-x^2}$ by Chebyshev polynomials of the first kind on a grid of nodes of the first kind

For the second example (see fig. 4), consider a function with high oscillation within an interval. To avoid repeating the earlier case and consider an alternative grid possibility, we will consider the expansion in Chebyshev polynomials of the first kind at the grid nodes of the first kind. The function in question

$$f_2(x) = \sin(\omega x)e^{-x^2}, \quad \omega = 50.$$

For this function, using the formula presented earlier, we calculate the matrix $\mathbf{A}$ and Due to the orthogonality of the Chebyshev polynomials, the Gram matrix also gets a diagonal structure

$$G = \tilde{A}^T\tilde{A} = \begin{pmatrix} n & 0 & 0 & \cdots & 0 \\ 0 & \frac{n}{2} & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \cdots & 0 \\ 0 & 0 & 0 & \frac{n}{2} & 0 \\ 0 & 0 & 0 & 0 & \frac{n}{2} \end{pmatrix}$$

After this, we multiply the vector of values by the transposed matrix and calculate the coefficients

$$c_k = (G^{-1})_{kk}\tilde{f}_k,$$

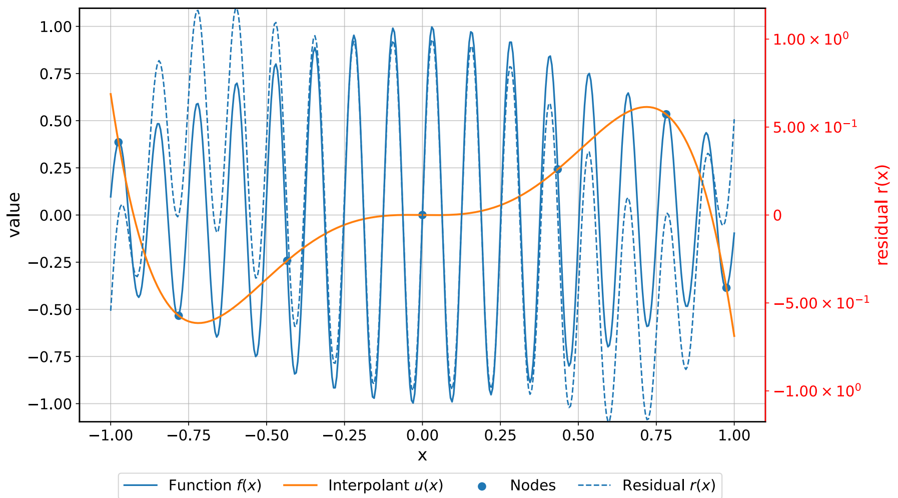

Figure 5: Interpolation of function $f_2(x) = \sin(\omega x)\, e^{-x^2}$ by Chebyshev polynomials of the first kind on a grid of 7 nodes of the first kind

Since this function is characterized by rapid oscillations within the interval, the interpolation task becomes significantly more complex. For $n = 7$, the interpolant is unable to accurately reproduce all the function's oscillations, resulting in a significant error of $\max|r(x)| = 1.176$. This is explained by the fact that the function's frequency ($\omega = 50$) is high, and its adequate reconstruction requires a larger number of basis functions.

As the number of nodes n increases, the interpolation polynomial begins to more accurately reproduce the oscillation structure, and the residual value decreases. Below is a graph where $n = 59$. At this value, the interpolant practically coincides with the function constructed analytically, and the residual is $\max|r(x)| = 1.007 \times 10^{-2}$.

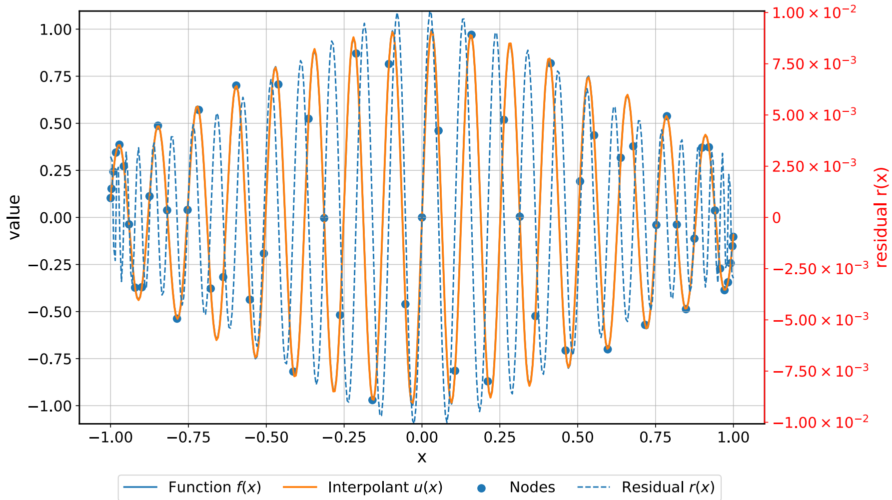

Figure 6: Interpolation of function $f_2(x) = \sin(\omega x)\, e^{-x^2}$ by Chebyshev polynomials of the first kind on a grid of 59 nodes of the first kind

This shows that the accuracy of the spectral method directly depends on the consistency of the number of nodes with the frequency structure of the function.

Interpolation of function $f_4(x) = |x - a|$ by Chebyshev polynomials of the second kind on a grid of nodes of the first kind

Both functions considered previously were smooth, and the question arises whether this method will perform equally well when considering a nonsmooth function. For this purpose, let us take as an example

$$f_4(x) = |x - a|, \quad a = 0.3.$$

For this function, we use the expansion in Chebyshev polynomial of the second kind on a grid of nodes of the first kind.

Using the algorithm described earlier, we calculate the matrix A and, since in this case we are considering polynomials of the second kind, we additionally multiply it by the weight $\tilde{A}_{kj} = \sqrt{w_k}\, U_j(x_k)$.

After this, we calculate the Gram matrix, which in this case also turns out to be diagonal

$$G = \tilde{A}^T \tilde{A} = \begin{pmatrix} \frac{n+1}{2} & 0 & 0 & \cdots & 0 \\ 0 & \frac{n+1}{2} & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \cdots & 0 \\ 0 & 0 & 0 & \frac{n+1}{2} & 0 \\ 0 & 0 & 0 & 0 & \frac{n+1}{2} \end{pmatrix}$$

As a result, the expansion coefficients are still calculated quite simply, despite the fact that the problem under consideration is nonsmooth.

$$c = (G^{-1})\tilde{f} = \frac{1}{4}\tilde{f}$$

The comparison of the interpolant graph with the analytical graph has the following form (see fig. 7).

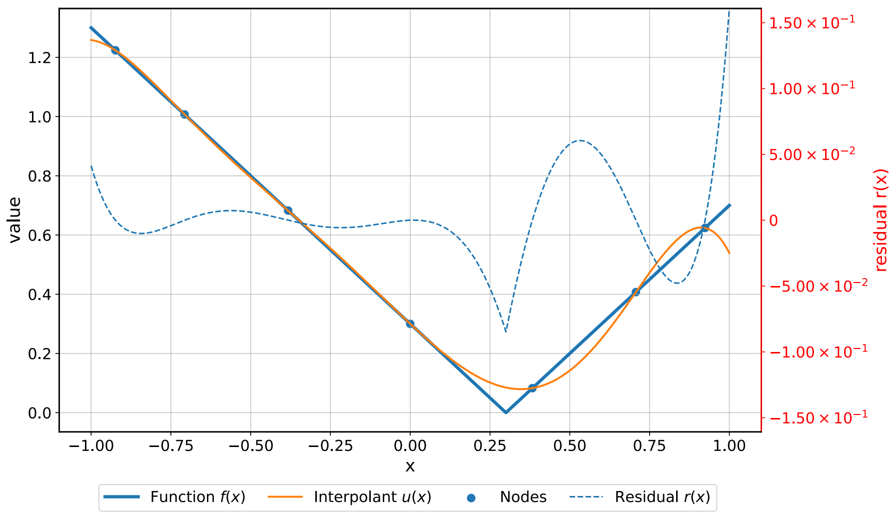

Figure 7: Interpolation of function $f_4(x) = |x - a|$ by Chebyshev polynomials of the second kind on a grid of 7 nodes of the first kind

In this case, the interpolated function is nonsmooth (it has a breakpoint at $x = a$), which significantly affects the accuracy of the spectral decomposition. The plot shows that the interpolant approximates the function well in smooth regions, but noticeable fluctuations occur near the discontinuity point of the derivative, and the residual value becomes $\max |r(x)| = 1.608 \times 10^{-1}$. Therefore, for the plot below, we will consider the case with $n = 26$ and see if the solution to the problem improves with an increase in the number of nodes, as was the case in the earlier examples.

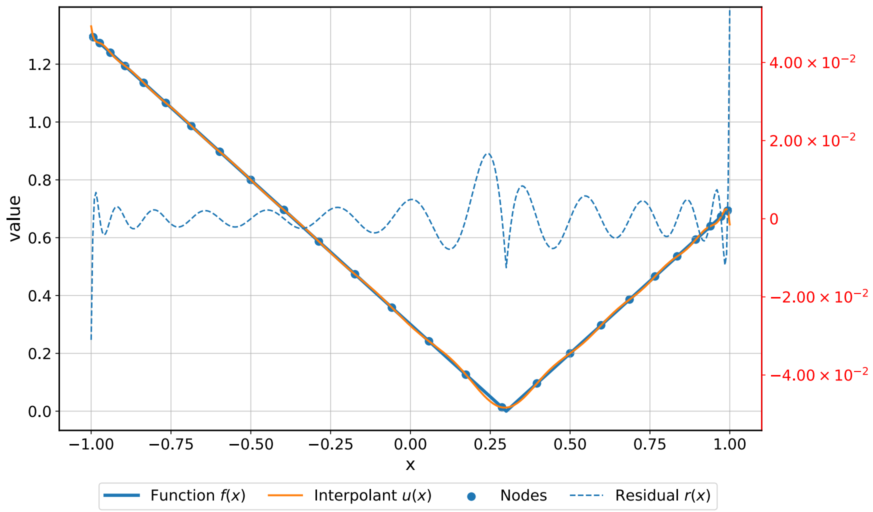

Figure 8: Interpolation of function $f_4(x) = |x - a|$ by Chebyshev polynomials of the second kind on a grid of 26 nodes of the first kind

The plot above shows that increasing the number of nodes n leads to an improvement in the approximation, as well as a decrease in the overall residual to $\max|r(x)| = 1.608 \times 10^{-1}$. Thus, even for non-smooth functions, the spectral method is still effective but requires a larger number of nodes in the vicinity of singular points to achieve high accuracy.

6. Conclusion

The article focuses on methods for calculating interpolation coefficients for functions using spectral collocation methods on Chebyshev–Gauss and Chebyshev–Lobatto grids. In all collocation methods used, the problem of calculating the coefficients of the interpolant expansion in basis functions (Chebyshev polynomials) using its values at the collocation points is reduced to solving a SLAE. The paper demonstrates that the procedure for solving a SLAE can be reduced to a set of simple arithmetic operations of addition and multiplication of the interpolant values at the collocation points by the matrix elements of the Chebyshev matrix with equal success for any combination of Chebyshev polynomials of the first or second kind on Chebyshev collocation grids.

This paper investigates the problem of fast, exact, and, most importantly, robust computation of spectral representations of functions on Chebyshev grids, based on the polynomial collocation method. Both Chebyshev polynomials T_n of the first kind and Chebyshev polynomials U_n of the second kind were considered as basis functions. Polynomials of the first kind T_n are more often used in function approximation since they ensure minimal error in the uniform norm L_∞. Polynomials of the second kind U_n are less commonly used for direct interpolation, but are indispensable in calculating integrals and solving ODEs, where the weight function

$\sqrt{1-x^2}$ corresponding to U_n naturally arises from the physical formulation of the problem.

Particular attention was paid to the consideration of interpolation processes on special non-uniform grids, the Chebyshev–Gauss grids and Chebyshev–Lobatto grids. Gauss nodes, coinciding with the roots of Chebyshev polynomials of the first kind, are found strictly within the interval $(-1, 1)$. Finding the coefficients by the collocation method on such a grid results in the highest possible algebraic accuracy in solving the integration problem. Lobatto nodes, at which the corresponding Chebyshev polynomial takes extreme values, including the boundaries of the closed interval $[-1, 1]$. Approximation of a function by the collocation method using a grid of this type provides a slightly lower approximation accuracy in the center of the interval compared to a Gauss grid. However, Chebyshev–Lobatto grids are often used in solving boundary value problems with strictly specified solution values at the boundaries of the interval, since they have the extreme points of the computational grid.

By applying minor preliminary transformations to the Chebyshev matrix in each of the four collocation methods, the Gram matrix of the resulting SLAE got a diagonal structure, and the expansion coefficients were calculated by element-by-element multiplication, rather than solving the full system of linear equations. Thus, it was shown that the choice of special interpolation grids can significantly simplify the computational complexity often associated with solving SLAEs with completely filled matrices [3].

The modified collocation methods discussed here allow for the computation of expansion coefficients for interpolated functions to be reduced to multiplying the Chebyshev matrix by a vector of function values at grid points. Using the discrete orthogonality of modified Chebyshev matrices when calculating interpolation coefficients in series expansions in polynomials of both the first and second kind ensures exponential convergence of the collocation method in each case, using both grid types.

The paper considers examples of solving interpolation problems for both smooth and non-smooth functions. High accuracy is achieved even with a small number of terms in the approximating series. For example, when studying the function $f_1(x) = e^{\alpha(x^2-1)}$ an increase in the number of nodes from $n = 7$ to $n = 15$ reduced the value of the maximum residual by several orders of magnitude, which is consistent with theoretical expectations [4]. It was also shown that for non-smooth functions the convergence rate is still high, but this requires a larger number of nodes [6]. Thus, with high function complexity, it is necessary to take a larger value of the parameter n, which is consistent with theoretical results on spectral convergence for smooth functions and slower convergence for non-smooth ones [6, 28].

The developed approach to calculating the coefficients of the expansion of functions in Chebyshev polynomials of the first and second kind on Chebyshev–Gauss and Chebyshev–Lobatto grids demonstrates a combination of high accuracy and computational efficiency, which makes it a promising tool not only for approximation problems, but also for the numerical solution of differential and integro-differential equations in engineering and scientific applications.

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