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AN OPTIMIZED LANCZOS TAU-METHOD

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Abstract. The paper puts forward an effective algorithm for producing approximate polynomial solutions for linear ordinary differential equations (LODEs) and sets of LODEs with polynomial coefficients and polynomial right-hand side functions. The algorithm is an upgraded version of the Lanczos Tau-method and provides the optimal deviation of the approximate solution from the exact one according to the minimax norm for a given interval. With minor modification, the algorithm allows one to find approximate expressions for the derivatives of the exact solutions with sufficiently greater accuracy than the derivatives of the approximate solutions are capable of providing that.

Keywords: minimax norm, Chebyshev polynomial, optimal approximation, linear ordinary differential equation, Tau-method

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ОПТИМИЗИРОВАННЫЙ ТАУ-МЕТОД ЛАНЦОША

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Аннотация. В статье обсуждается эффективный алгоритм получения приближенных полиномиальных решений для линейных обыкновенных дифференциальных уравнений и систем линейных обыкновенных дифференциальных уравнений с полиномиальными коэффициентами и полиномиальными правыми функциями. Алгоритм является усовершенствованной версией тау-метода К. Ланцоша и дает возможность получать оптимальное отклонение приближенного решения от точного в соответствии с минимаксной нормой для заданного отрезка. При незначительной модификации алгоритм позволяет находить приближенные выражения для производных точных решений с существенно большей точностью, чем способны обеспечивать производные приближенных решений.

Ключевые слова: минимаксная норма, полином Чебышева, оптимальная аппроксимация, линейное обыкновенное дифференциальное уравнение, тау-метод

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Introduction

The Lanczos Tau-method[1] allows to obtain approximate polynomial solutions for linear ordinary differential equations (LODEs) with polynomial coefficients and polynomial right-hand functions [1, 2]. These solutions should have maximum accuracy in a finite interval under consideration in accordance with the minimax norm, which is the opposite of approximation by ordinary least squares and/or approximation by series of orthogonal polynomials of various types [3–5].

This article discusses the reasons why polynomial solutions obtained using the original Lanczos algorithm may turn out to be suboptimal and suggests effective ways to improve the algorithm. General theoretical considerations are supported by numerical examples.

Initially, the Tau-method was proposed in [1] and subsequently described in detail in monograph [2] with a large number of illustrative examples. The basic mathematical definitions allowing to rigorously describe the method are given in [6]. A case considered in [7] concerns an interval divided into small segments, subsequently applying the Tau-method to each small segment to obtain a smooth and accurate approximate piecewise polynomial solution.

Another approach to improving the accuracy of this method is described in [8]. Recurrent schemes of the Tau-method, when the degree of the approximating polynomial is increased in steps, without recalculating it from zero, are considered in [9, 10]. The errors of approximate solutions are analyzed in [11, 12]. Extensions of the Tau-method to linear differential equations with coefficients differing from polynomial to nonlinear differential equations, partial differential equations, etc., are discussed in [13–15].

Revived interest in techniques for constructing approximate solutions of ODEs, systems of integral equations and other objects can be traced in recent publications. The Lanczos Tau-method is also used, but with the construction of a shifted Legendre basis for solving time-delay systems [16]; the approximation of differential operators is applied (the same as in our paper) with shifted Chebyshev polynomials [17], expansions of functions with respect to Hermite and Laguerre polynomials are presented [18].

In addition, the special Tau Toolbox was developed[2], in particular for solving ODEs (including nonlinear ones) and their systems, as well as integral equations [19–21]. Applications of this toolbox to expansion of solutions with respect to Sobolev polynomials and solutions of singular integral equations can be found in [22, 23]. The coefficients of approximating formulas are sought in [24] when the Chebyshev alternation is reached. This approach is used in the approximation of Fermi–Dirac functions based on an iterative procedure.

More recent studies consider Chebyshev approximations of functions [25, 26]; several textbooks deal with a wider range of issues related to the search for approximate solutions and substantiation of their properties [27–29].

Thus, interest in this major research problem does not weaken.

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[1] The name Tau-method was proposed and introduced by Cornelius Lanczos (a Hungarian physicist and mathematician) in [1]: the additional free terms for the Chebyshev polynomials on the right-hand side of differential equations were denoted with the subscripts τ.

[2] The package can be downloaded from the website https://bitbucket.org/tautoolbox/tautoolbox/src/main/.

The Tau-method was originally formulated as a way to approximate special functions of mathematical physics that could be expressed using ODEs. This method has become a powerful and accurate tool for numerical solution of complex differential and functional equations. The approach proposed by Lanczos is to approximate the solution of a given problem by calculating the exact solution of some approximate problem close to the original one. The solution of the differential equation along this path is approximated by a polynomial which is an exact solution to the differential equation obtained by adding the polynomial terms of the perturbation to its right-hand side. The perturbation terms are chosen so as to guarantee the existence of an analytical polynomial solution to the perturbed equation.

If the coefficients of the equation and/or the initial conditions and/or the boundaries of the interval depend on any parameters, then the output is an algebraic expression depending on these parameters. This is an undoubted advantage of the Tau-method, compared with classical numerical methods that produce individual solutions for fixed numerical values of parameters. The method can greatly simplify analysis, allowing to optimize solutions to parameter-dependent differential equations.

The following section contains various definitions and theorems to be used further for this study.

The section 'Example solution of equation by Tau-method' illustrates the steps of the Lanczos Tau-method; here a linear differential equation with polynomial coefficients and a known analytical non-polynomial solution is solved.

The section 'Difference between errors and residuals' analyzed the fundamental difference between the error (the discrepancy between the exact and approximate solutions) and the differential residual (the parasitic value on the right-hand side of the differential equation after substituting the approximate solution). Minimization of the differential residual is not equivalent to minimization of the error, and therefore Chebyshev polynomials or some other orthogonal polynomials used to minimize the differential residual do not provide an optimal approximate solution.

The following section describes an optimized Tau-method for solving reduced LODEs with polynomial coefficients. The integral form of a LODE and Picard's theorem make it possible to prove the statement that the residual of integral form is proportional to the error of the approximate solution. Therefore, if the perturbation of integral form is the sum of Chebyshev polynomials, the approximate solution obtained by the Tau-method is close to optimal. The optimized Tau-method introduces perturbations both to the right-hand side of the differential equation and to the initial conditions of the approximate solution (the latter differs significantly from the original Tau-method).

The section 'Discussion' compares the approaches to the problem and analyzes the advantages of the proposed modification of the method.

The main results are summarized in Conclusion.

Necessary definitions and general theorems

This section contains definitions and general theorems used later in this study. Details and proofs of the corresponding statements can be found in books [3–5].

Definition 1. A polynomial of the form

$$P(x) = a_0 + a_1 x + \ldots + a_n x^n$$

of degree n is the minimax approximation of the given function $f(x)$ with the given weight $w(x) \neq 0$ on the given interval $x \in [x_a, x_b]$, if $P(x)$ is the solution to the variational problem

$$\max_{x\in[x_a,x_b]} \left| w(x)\left(f(x) - P(x)\right)\right| \to \min \tag{1}$$

where minimization is performed over all possible sets of coefficients a_0, a_1, ..., a_{n-1}, a_n.

Definition 2. A reduced polynomial of the form

$$P(x) = a_0 + a_1 x + \ldots + a_{n-1} x^{n-1} + x^n$$

of degree n is called the polynomial of least deviation from zero on the given interval $x \in [x_a, x_b]$ with the given weight $w(x) \neq 0$ if $P(x)$ is the solution to the variational problem

$$\max_{x\in[x_a,x_b]} \left| w(x) P(x)\right| \to \min, \tag{2}$$

where minimization is performed over all possible sets of coefficients a_0, a_1, ..., a_{n-1}.

The lower part $a_0 + a_1 x + ...+ a_{n-1}x^{n-1}$ of a polynomial of degree n of least deviation from zero is a polynomial of degree $n - 1$ providing a minimax approximation (solution to variational problem (1)) for the function $f(x) = -x^n$ with the weight $w(x)$.

Definition 3. A set of m points

$$x_1 < x_2 < \ldots < x_m$$

is called a Chebyshev alternation of size m for a function $h(x)$ on the interval $[x_a, x_b]$ if the points $x_k \in [x_a, x_b]$ are alternating local minima and maxima of $h(x)$ with equal absolute values, so that

$$h(x_k) = (-1)^k \varepsilon \text{ and } |\varepsilon| = \max|h(x)| \text{ for } x \in [x_a, x_b].$$

Theorem 1 (de la Vallée Poussin theorem). *Suppose there is a polynomial $Q(x)$ of degree n, a function $f(x)$, an interval $[x_a,x_b]$ and a weight function $w(x) \neq 0$. Let us also assume that there are $n + 2$ points (de la Vallée Poussin alternation)*

$$x_a \le x_1 < x_2 < \ldots < x_{n+2} \le x_b,$$

in which the expression $w(x)[f(x) - Q(x)]$ has nonzero values with alternating signs:

$$+\lambda_1, -\lambda_2, \ldots, + (-1)^{n+2} \lambda_{n+2}$$

(it is assumed that $\lambda_k > 0$ for $\forall k$)).

If λ is the minimax deviation from zero for

$$w(x)\ [f(x) - P(x)],$$

where the optimal polynomial $P(x)$ is the solution of the variational problem (1), then

$$\lambda \ge \min\{\lambda_1, \lambda_2, \ldots, \lambda_{n+2}\}.$$

If the given points x_k are also local minima and maxima forw(x)$[f(x) - Q(x)]$, then

$$\lambda \le \max\{\lambda_1, \lambda_2, \ldots, \lambda_{n+2}\}.$$

Theorem 2 (Chebyshev's alternation theorem). *If there exists a Chebyshev alternation of size $n + 2$ on the interval $[x_a, x_b]$ for the function w(x) $[f(x) - P(x)]$, where w(x) $\neq 0$ and $f(x)$ are the given functions, and $P(x)$ is a polynomial of degree n, then this polynomial $P(x)$ is the only solution to variational problem (1). If the functions $w(x) \neq 0$ and $f(x)$ are continuous on the interval $[x_a,x_b]$, then variational problem (1) has a unique solution $P(x)$, and this solution satisfies the condition of Chebyshev's theorem, i.e., there is a Chebyshev alternation of dimension $n + 2$ on the interval $[x_a,x_b]$ for the function $w(x)[f(x) - P(x)]$.*

Theorem 3 (Chebyshev criterion). *If a Chebyshev alternation of size $n + 1$ exists for a function $w(x)P(x)$ on the interval $[x_a,x_b]$, where $w(x) \neq 0$* is *the given function, and $P(x)$ is a polynomial of degree n with the leading coefficient equal to unity, then the polynomial P(x) is a unique solution to the variational problem (2), i.e., the polynomial of least deviation from zero. If the function $w(x) \neq 0$ is continuous on the interval $[x_a,x_b]$, then variational problem (2) has a unique solution, and this solution satisfies the Chebyshev criterion, i.e., a Chebyshev alternation of size $n + 1$ exists for function $w(x)P(x)$ on the interval $[x_a,x_b]$.*

Algorithms allowing to calculate polynomials for minimax approximations and polynomials of least deviation from zero for the given weight $w(x) \neq 0$ on the given interval $[x_a,x_b]$ are considered in [30–32].

Definition 4. Polynomials $T_n(x)$ of degree n, defined as

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

for $-1 \le x \le +1$ are called first-kind Chebyshev polynomials.

According to Definition 2 and Theorem 3, the polynomials $T_n(x)/2^{n-1}$ are polynomials of degree n that deviate least from zero on the interval $x \in [-1,+1]$ with weight $w(x) = 1$. The deviation is equal to $1/2^{n-1}$.

Definition 5. Let there be an ordinary differential equation of the form

$$L[x(t)] = 0,$$

where $L[x(t)]$ is a certain differential operator.

If the following equality holds true for the trial function $x(t)$:

$$L[x(t)] = Q(t),$$

then $Q(t)$ is called the differential residual of $x(t)$.

Definition 6. Let there be an integral equation

$$x(t) = K[x(t)],$$

equivalent to the differential equation

$$L[x(t)] = 0,$$

where $K[x(t)]$ a certain integral operator.

If the following equality holds true for the trial function $x(t)$:

$$x(t) - K[x(t)] = R(t),$$

then $R(t)$ is called the integral residual of $x(t)$.

Definition 7. Let there be an ordinary differential equation

$$L[x(t)] = 0,$$

such that $x^*(t)$ is the exact solution of the equation. If $x(t)$ is an approximate solution of the equation, then the difference

$$\Delta x(t) = x(t) - x^*(t)$$

is called the error of the approximate solution $x(t)$.

Remark 1. Differential residuals, integral residuals and errors for systems of ODEs are introduced similarly.

Example solution of equation by Tau-method

The Lanczos method gives approximate polynomial solutions on a certain fixed interval for LODEs with polynomial coefficients and polynomial right-hand sides of the form

$$L[x(t)] = x^{(n)}(t) + a_1(t)x^{(n-1)}(t) + \ldots + a_{n-1}(t)x'(t) + a_n(t)x(t) - f(t) = 0,$$

where $a_k(t)$, $f(t)$ are polynomials; $x(t)$ is an unknown function.

For illustration, consider a simple example:

$$L[x(t)] = x''(t) + tx'(t) + 2x(t) = 0,$$
$$x(0) = 0,\ x'(0) = 1. \tag{3}$$

The exact solution of Eq. (3) is $x^*(t) = t\exp(-t^2/2)$. Suppose that the exact solution is unknown and it is necessary to find an approximate solution to problem (3) at $0 \le t \le 4$. The Weierstrass approximation theorem (see, for example, monograph [33]) guarantees that any continuous function can be approximated on a fixed interval of finite size with arbitrarily high accuracy by a polynomial of the appropriate degree. This statement serves as the basis for finding an approximate solution in the form of a polynomial for the given problem.

We search for an approximate solution to problem (3) as a 7th-degree polynomial with indefinite coefficients b_k:

$$x(t) = b_0 + b_1 t + b_2 t^2 + \ldots + b_7 t^7. \tag{4}$$

After substituting expression (4) into Eq. (3), the right-hand side (differential residual) turns out to be a polynomial:

$$Q(t) = (2b_0 + 2b_2) + (3b_1 + 6b_3)t + (4b_2 + 12b_4)t^2 + (5b_3 + 20b_5)t^3 +$$
$$+ (6b_4 + 30b_6)t^4 + (7b_5 + 42b_7)t^5 + 8b_6 t^6 + 9b_7 t^7. \tag{5}$$

We need to bring differential residual (5) as close to zero as possible; for example, by satisfying the condition $Q(t) \equiv 0$. However, this is possible only when the exact solution of the equation is a polynomial of the required (or lower) degree. The statement 'bring the residual as close to zero as possible' is not clearly defined and cannot be regarded as unambiguous in a mathematical sense. For example, we set as many coefficients of the lower-degree terms in residual (5) as possible equal to zero, provided that some coefficients are used to satisfy the initial conditions. This is sufficient for residual (5) to exclude terms with multipliers 1, t, t^2, t^3, t^4, t^5 and even t^6. Then the solution is as follows:

$$b_0 = b_2 = b_4 = b_6 = 0,\ b_1 = 1,\ b_3 = -1/2,\ b_5 = 1/8,\ b_7 = -1/48,$$
$$Q(t) = -3/16t^7. \tag{6}$$

As expected, this result is a truncated Taylor series for the function $t\exp(-t^2/2)$. Fig. 1 shows a comparison of the exact solution with the approximate polynomial solution (4) with coefficients (6) for $t \in [0,4]$. Obviously, this solution is unsatisfactory, despite the high degree of the polynomial.

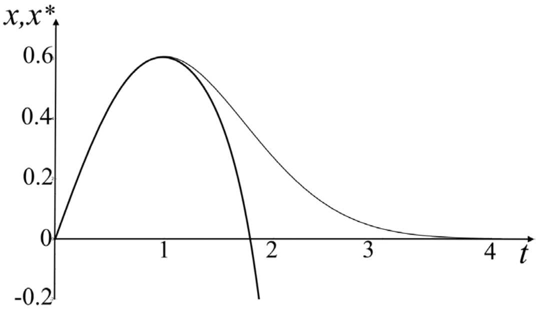

Fig. 1. Exact ($x^*(t)$) and approximate ($x(t)$) solutions of differential equation (3) (thin and bold lines, respectively); the coefficients of the polynomial $x(t)$ are determined by Eqs. (6)

One of the possible reasons for this failure is that although the differential residual $Q(t) = -3t^7/16$ is small near the point $t = 0$, this residual is unreasonably large in the vicinity of the point $t = 4$. Apparently, if we require that the residual be approximately the same over the entire interval, then we can expect a significantly better result.

The first step proposed by Lanczos *is* to remove the ill-defined empirical conditions. In the new formulation of the problem, it is necessary to find the coefficients b_0, $b_1 - b_7$, τ_6, τ_7 for which function (5) satisfies the conditions

$$x(0) = 0,\ x'(0) = 1,\ L[x(t)] \equiv \tau_6 t^6 + \tau_7 t^7.$$

The problem has not actually changed, but now the system of equations is well-defined from an algebraic standpoint. The corresponding SLAE has a unique solution. Naturally, this solution coincides with solution (6).

The next important step proposed by Lanczos consists in replacing the differential residual $\tau_6 t^6 + \tau_7 t^7$ (i.e., a function that is small at one end of the interval but large at the other end) with a differential residual

$$\tau_6 \overline{T}_6(t) + \tau_7 \overline{T}_7(t),$$

where $\overline{T}_6(t)$ and $\overline{T}_7(t)$ are transformed Chebyshev polynomials $T_6(t)$ and $T_7(t)$ of the corresponding degree [2, 34, 35].

These polynomials are rescaled from $t \in [-1, +1]$ to $t \in [0, 4]$ and deviate least from zero on the interval $t \in [0.4]$:

$$\tau_6 \overline{T}_6(t) + \tau_7 \overline{T}_7(t),$$

$$\overline{T}_6(t) = T_6\left(\frac{t}{2} - 1\right),\ \overline{T}_7(t) = T_7\left(\frac{t}{2} - 1\right),$$

$$T_6(\tau) = 32\tau^6 - 48\tau^4 + 18\tau^2 - 1,$$

$$T_7(\tau) = 64\tau^7 - 112\tau^5 + 56\tau^3 - 7\tau.$$

Now the differential residual $Q(t)$ on the right-hand side of the equation is approximately the same at all points of the interval under consideration. Then it is logical to assume that the error of the approximate solution is also approximately the same over the entire interval. This hypothesis is supported by the fact that the error of the approximate solution is zero at all points of the interval provided that the residual $Q(t)$ is zero at all of its points. However, minimization of the residual does not necessarily mean minimization of the error (see the example below).

Solution (4), obtained for Eq. (3) using the Lanczos Tau-method, contains the following coefficients:

$$b_0 = 0,\ b_1 = 1.000000000,\ b_2 \approx 0.052400600,\ b_3 \approx -0.880052000,$$
$$b_4 \approx 0.442647000,\ b_5 \approx -0.091658100, \quad (7)$$
$$b_6 \approx 0.006894820,\ b_7 \approx -0.000023572.$$

Fig. 2 illustrates the discrepancy between the exact and approximate polynomial solutions (4) with coefficients (7) obtained using the Lanczos Tau-method. The approximate solution $x(t)$ lies in the range of 0–0.6 with the maximum error on the interval $t \in [0.4]$ equal to 0.012. The graphs of the exact and approximate solutions are virtually indistinguishable. Fig. 2 shows the graphs for error and differential residual. It can be seen that the accuracy of the approximate solution obtained using the Lanczos Tau-method is satisfactory.

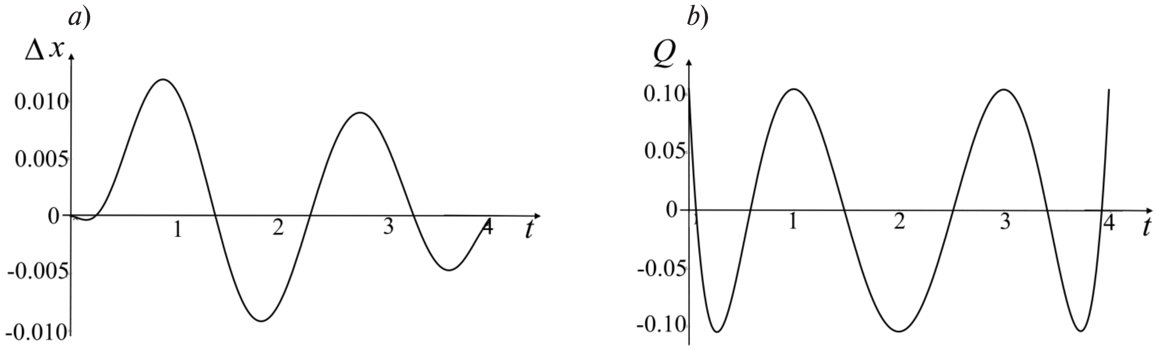

Fig. 2. Error of approximate solution obtained by Lanczos Tau-method (*a*) and its differential residual (*b*)

Monograph [34] shows that expanding the approximate solution into a truncated Chebyshev series often yields higher accuracy than the Lanczos method. However, approximate solutions obtained using the truncated Chebyshev series also do not guarantee the highest possible accuracy. The goal of this study is to create a modification of the Lanczos Tau-method providing the highest possible accuracy of the approximate solution.

Indeed, a small (with respect to the minimax norm) differential residual in the differential equation does not mean a small minimax error of the solution. As an example, consider the equation $y''(t) + y(t) = 0$ with an exact solution

$$y^*(t) = c_1\cos t + c_2\sin t$$

and the equation $z''(t) + z(t) = \varepsilon\sin t$ with the exact solution

$$z^*(t) = c_1\cos t + c_2\sin t - \varepsilon(t\cos t - \sin t)/2.$$

No matter how small the differential residual $Q(t) = \varepsilon\sin t$ is in the second equation, the difference between these two solutions with the same initial conditions becomes arbitrarily large as the interval $t \in [0, T]$ increases.

Difference between errors and residuals

The error $\Delta x(t)$ is the difference between the exact solution $x^*(t)$ and the approximate solution $x(t)$. The differential residual $Q(t)$ is the deviation of the right-hand side of the differential equation after an approximate solution is substituted. The theorem on the unique solution for ODEs states:

"*If the differential residual is zero everywhere, then the error is zero everywhere, and vice versa.*"

The Lanczos Tau-method is an attempt to make the differential residual as close to zero as possible, assuming that this keeps the error as close to zero as possible. As proved above, this statement is incorrect.

To find the relationship between the error and the differential residual, it is necessary to use the integral form of the equation. Suppose that there is an equation

$$y^{(n)}(t) + c_1(t)y^{(n-1)}(t) + \ldots + c_n(t)y + c(t) = 0, \tag{8}$$

where $c_1(t)$, $c_2(t)$, ..., $c_n(t)$ and $c(t)$ are continuous on the interval $t \in [t_0, T]$. Eq. (8) is equivalent to the equation

$$\begin{gathered} y(t) = y_0 + y_0'(t-t_0) + \ldots + y_0^{(n-1)}\frac{(t-t_0)^{n-1}}{(n-1)!} - \\ -\int_{t_0}^{t}\ldots\int_{t_0}^{t}\left[c_1(t)y^{(n-1)}(t) + \ldots + c_n(t)y(t) + c(t)\right]dt\ldots dt, \end{gathered} \tag{9}$$

where $y(t_0) = y_0$, $y'(t_0) = y'_0$, ..., $y^{(n-1)}(t_0) = y^{(n-1)}{}_0$ are the initial conditions for Eq. (8).

Picard's theorem [36] on the existence and uniqueness of a solution to a LODE uses, in particular, a recurrent sequence of functions $y_k(t)$ defined by the equalities

$$y_{k+1}(t) = N[y_k(t)], \tag{10}$$

where $N[y(t)]$ is the integral operator on the right-hand side of expression (9).

Regardless of the initial function $y_0(t)$ and the size of the considered finite interval $t \in [t_0, T]$, iterations quickly converge to the solution of integral equation (9), i.e., to the solution $y(t)$ of differential equation (8). The given solution is unique and definite for any $t \in [t_0, T]$.

Analyzing the proof of Picard's theorem, we find that

$$\max_{t\in[t_0,T]}\left|y(t) - y_k(t)\right| \le C\max_{t\in[t_0,T]}\left|y_{k+1}(t) - y_k(t)\right|, \tag{11}$$

where the constant C is determined only by the coefficients of Eq. (8) and the interval $[t_0, T]$. A more accurate estimate leads to the equality $C = C_0/k!$

Importantly, the constant C in Eq. (11) does not depend on the choice of initial function $y_0(t)$, chain of functions $y_k(t)$ or solution $y(t)$.

This result can be formulated as follows.

Theorem 4 (about the integral residual). *Assume that $y(t) = N[y(t)]$ is the integral equation (9) obtained from differential equation (8); $y(t)$, $z(t)$ are the exact and approximate solutions of Eqs. (8) and (9), respectively; $R(t)$ is the integral residual for $z(t)$, given by the relation*

$$z(t) = N[z(t)] + R(t). \tag{12}$$

Then the error $y(t) - z(t)$ satisfies the relation

$$\max_{t\in[t_0,T]}\left|y(t) - z(t)\right| \le C\max_{t\in[t_0,T]}\left|R(t)\right|, \tag{13}$$

where the constant C is determined only by the coefficients of Eq. (8) and the interval $[t_0, T]$.

P r o o f. Integration by parts gives the relations

$$\int_{t_0}^{t} c_{n-1}(t)\,y'(t)\,dt = c_{n-1}(t)\,y(t) - c_{n-1}(t_0)\,y(t_0) - \int_{t_0}^{t} c'_{n-1}(t)\,y(t)\,dt,$$

$$\begin{aligned}
&\int_{t_0}^{t} dt\left(\int_{t_0}^{t} c_{n-2}(t)\,y''(t)\,dt\right) = \int_{t_0}^{t} dt\left(c_{n-2}(t)\,y'(t) - c_{n-2}(t_0)\,y'(t_0) - \int_{t_0}^{t} c'_{n-2}(t)\,y'(t)\,dt\right) = \\
&= c_{n-2}(t)\,y(t) - c_{n-2}(t_0)\,y(t_0) - \int_{t_0}^{t} c'_{n-2}(t)\,y(t)\,dt - c_{n-2}(t_0)\,y'(t_0)\frac{(t-t_0)}{1!} - \\
&-\int_{t_0}^{t} dt\left(c'_{n-2}(t)\,y(t) - c'_{n-2}(t_0)\,y(t_0) - \int_{t_0}^{t} c''_{n-2}(t)\,y(t)\,dt\right) = \\
&= c_{n-2}(t)\,y(t) - \int_{t_0}^{t} 2c'_{n-2}(t)\,y(t)\,dt + \int_{t_0}^{t} dt\left(\int_{t_0}^{t} c''_{n-2}(t)\,y(t)\,dt\right) - \\
&-c_{n-2}(t_0)\,y(t_0) - c_{n-2}(t_0)\,y'(t_0)\frac{(t-t_0)}{1!} + c'_{n-2}(t_0)\,y(t_0)\frac{(t-t_0)}{1!},
\end{aligned} \tag{13}$$

$$\int_{t_0}^{t} dt\left(\int_{t_0}^{t} dt\left(\int_{t_0}^{t} c_{n-3}(t)\,y'''(t)\,dt\right)\right) = \ldots$$

Integral equation (9) is transformed into an equivalent integral equation of the form

$$y(t) = H(t) + \int_{t_0}^{t} dt\left(h_1(t)\,y(t) + \int_{t_0}^{t} dt\left(h_2(t)\,y(t) + \ldots + \int_{t_0}^{t} dt\left(h_n(t)\,y(t) + c(t)\right)\right)\right),$$

where $h_k(t)$ are some continuous functions (e.g., polynomials) defined by coefficients $c_k(t)$ after integration by parts; $H(t)$ *is* a polynomial of degree $n - 1$ with the coefficients given by complex expressions involving the values of the known functions (coefficients of the equation and their derivatives) at $t = t_0$ and the known initial conditions for $y(t)$.

Importantly, $H(t)$ does not depend on the unknown solution $y(t)$.

Iterations

$$y_{k+1}(t) = H(t) + \int_{t_0}^{t} dt\left(h_1(t)\,y_k(t) + \int_{t_0}^{t} dt\left(h_2(t)\,y_k(t) + \ldots + \int_{t_0}^{t} dt\left(h_n(t)\,y_k(t) + c(t)\right)\right)\right)$$

converge quickly under any initial condition $y_0(t)$. To prove this, we introduce the notations

$$\Delta y_k(t) = y_{k+1}(t) - y_k(t),\; M = \max_{t\in[t_0,T]}\left|\Delta y_0(t)\right|,\; H_k = \max_{t\in[t_0,T]}\left|h_k(t)\right|.$$

The iterations for $\Delta y_k(t)$ take the form

$$\Delta y_{k+1}(t) = \int_{t_0}^{t} dt\left(h_1(t)\,\Delta y_k(t) + \int_{t_0}^{t} dt\left(h_2(t)\,\Delta y_k(t) + \ldots + \int_{t_0}^{t} h_n(t)\,\Delta y_k(t)\,dt\right)\right),$$

whence we obtain the following estimates for the interval $t \in [t_0, T]$:

$$|\Delta y_0(t)| \le M,$$

$$|\Delta y_1(t)| \le M(\Delta TH_1\Delta t + \Delta T^2 H_2 \Delta t^2/2! + \ldots + \Delta T^n H_n \Delta t^n/n!) \le MG\Delta t,$$

$$|\Delta y_2(t)| \le MG(\Delta TH_1\Delta t^2/2! + \Delta T^2 H_2 \Delta t^3/3! + \ldots) \le MG^2\Delta t^2/2!$$

. . . .

$$|\Delta y_k(t)| \le MG^k\Delta t^k/k!,$$

where $\Delta t = (t - t_0)/\Delta T$, $\Delta T = T - t_0$; $0 \le \Delta t \le 1$, G is a constant:

$$G = \Delta TH_1 + \Delta T^2 H_2 + \ldots + \Delta T^n H_n.$$

A sequence of iterative values

$$y_{k+1}(t) = y_0(t) + \Delta y_0(t) + \Delta y_1(t) + \ldots + \Delta y_k(t)$$

converges uniformly on the interval $t \in [t_0, T]$, since the sum of the increments $\Delta y_k(t)$ is majorized by uniformly absolutely-convergent series:

$$|\Delta y_0(t) + \Delta y_1(t) + \ldots + \Delta y_k(t)| \le |\Delta y_0(t)| + |\Delta y_1(t)| + \ldots +$$

$$+ |\Delta y_k(t)| + \ldots \le M \exp(G\Delta t).$$

Therefore, there is a limit $y_{k+1}(t) \to y(t)$; it gives the solution $y(t)$ of integral equation (9) and differential equation (8), as well as an error estimate:

$$|y(t) - y_0(t)| \le |\Delta y_0(t)| + |\Delta y_1(t)| + \ldots + |\Delta y_k(t)| + \ldots \le$$
$$\le M \exp(G\Delta t) \le MC, \tag{14}$$

although this may turn out to be a very rough estimate of the constant C used in inequality (12).

Let $y_0(t) = z(t)$, where $z(t)$ satisfies Eq. (12). Then the following equalities hold true:

$$y_1(t) = N[z(t)] = z(t) - R(t),\ \Delta y_0(t) = y_1(t) - y_0(t) = -R(t),$$

$$M = \max|\Delta y_0(t)| = \max|R(t)|.$$

Combining this relation with Eq. (14), we obtain relation (12).

Theorem 4 is proved.

This proof bears significant similarities to the proof of Picard's theorem for systems of LODEs [30], but with minor modifications. Inequality (13) means that in order to minimize the difference between the approximate solution $z(t)$ and the exact solution $y(t)$, we should minimize the modulus of the function $R(t)$ in Eq. (12). Returning from Eq. (9) to Eq. (8), equality (12) is transformed into equality

$$z^{(n)}(t) + c_1(t)z^{(n-1)}(t) + \ldots + c_n(t)z + c(t) = Q(t) = d^nR(t)/dt^n. \tag{15}$$

Eq. (15) shows that the differential residual for the Tau-method is the nth derivative of the error with an accuracy up to a constant factor (see inequality (13)). In particular, if the sum of Chebyshev polynomials is used as a perturbation for the right-hand side of differential equations, as is done in the original Lanczos method, then the error of the approximate solution is an n-fold integral of the sum composed of Chebyshev polynomials. Therefore, the error of the approximate solution for high-order differential equations may be far from the function deviating least from zero.

Similar statements are true for systems of LODEs with continuous coefficients.

Optimized Tau-method for solving differential equations

Suppose that there is a LODE (8) where the leading coefficient is equal to, and the remaining coefficients and the free term are polynomials of the independent variable. As discussed in the previous section, an optimal approximate solution is obtained by selecting the right-hand side in the form

$$R(t)=\sum_k \tau_k \overline{T}_{k+n}(t), \tag{16}$$

where $\overline{T}_{k+n}(t)$ are first-kind Chebyshev polynomials of least deviation from zero, with an argument scaled from the interval [-1, +1] to the interval $[t_0, T]$; τ_k are constants to be determined later.

The number of terms in sum (16) and the degrees of the polynomials correspond to the differential residual in the right-hand side of differential equation (8) after substituting an approximate polynomial solution with indefinite coefficients.

If the integral form

$$z(t)=y_0+y_0'(t-t_0)+\ldots+y_0^{(n-1)}\frac{(t-t_0)^{n-1}}{(n-1)!}+\sum_k \tau_k \overline{T}_{k+n}(t)-$$
$$-\int_{t_0}^{t}\ldots\int_{t_0}^{t}\left[c_1(t)z^{(n-1)}(t)+\ldots+c_n(t)z(t)+c(t)\right]dt\ldots dt. \tag{17}$$

is converted to a differential equation, the output signal is equal to

$$z^{(n)}(t)+c_1(t)z^{(n-1)}(t)+\ldots+c_n(t)z+c(t)=\sum_k \tau_k \overline{S}_k(t), \tag{18}$$

where the polynomials $\overline{S}_k(t)$ are defined as

$$\overline{S}_k(t)=d^n\overline{T}_{k+n}(t)/dt^n .$$

Similarly to the original Lanczos method, Eq. (18) allows to determine both the coefficients of the approximate solution $z(t)$ and the coefficients τ_k. In addition, analysis of Eq. (17) shows that the initial conditions of the approximate solution $z(t)$ should be calculated as

$$z_0^{(j)}=\left.\frac{d^j z(t)}{dt^j}\right|_{t=t_0}=y_0^{(j)}+\sum_k \tau_k \left.\frac{d^j \overline{T}_{k+n}(t)}{dt^j}\right|_{t=t_0}, \; j=0,\ 1,\ \ldots,\ n-1. \tag{19}$$

Combining Eqs. (19) and linear equations derived from Eq. (18), we can unambiguously find all the indefinite coefficients. This result can be formulated as follows.

Theorem 5. *Let the optimized Tau-method be obtained by combining relations (18) for the differential residual of the approximate solution $z(t)$ and relations (19) for the initial conditions of the approximate solution $z(t)$, where $\overline{S}_k(t)=d^n\overline{T}_{k+n}(t)/dt^n$ and $\overline{T}_{k+n}(t)$ are Chebyshev polynomials of degree $k+n$, recalculated from the interval $[-1,+1]$ to the interval $[t_0,T]$. Then the error of the approximate solution $z(t)$, calculated as an exact analytical solution of the perturbed problem (18), (19), satisfies the relation*

$$\max_{t\in[t_0,T]}\left|y(t)-z(t)\right|\le C\max_{t\in[t_0,T]}\left|\sum_k \tau_k \overline{T}_{k+n}(t)\right|\le C\sum_k |\tau_k|, \tag{20}$$

where the constant C in Eq. (20) is determined only by the coefficients of Eq. (8) and the interval $[t_0, T]$, and the approximate solution $z(t)$ obtained by this technique is close to the optimal minimax approximation of the exact solution y(t).

Proof. The statement of the theorem follows directly from Theorem 4 if the weighted sum of scaled first-kind Chebyshev polynomials is used as the integral residual. The final inequality in Eq. (20) follows from the fact that the minimax norm of each of the scaled Chebyshev polynomials on the interval under consideration equals unity.

Theorem 5 is proved

Remark 2. Strictly speaking, the sum of several scaled Chebyshev polynomials is not the polynomial that deviates least from zero on the interval under consideration, and therefore the approximate solution obtained differs from the optimal minimax approximation of the exact solution of the differential equation. The deviation of the error of the approximate solution from the error of the true minimax approximation to the exact solution $y(t)$ is determined by the de la Vallée Poussin theorem (see Theorem 1) after analysis of the local minima and maxima of the value of the right-hand side in inequality (20).

Remark 3. In the case when exact initial conditions are required, the polynomials $\overline{T}_{k+n}(t)$ are represented as

$$\overline{T}_{k+n}(t) = (t - t_0)^n T_n^*\left((t - t_0)/(T - t_0)\right),$$

where $T^*_n(t)$ are the polynomials deviating least from zero, with the weight t^n on the normalized interval $t \in [0,1]$.

This procedure gives a large error but allows to set accurate initial conditions. Algorithms for numerical calculation of polynomials are discussed in [25–27].

Example. Consider an approximate solution of problem (3) in the form of a polynomial

$$x(t) = c_0 + c_1 t + c_2 t^2 + c_3 t^3 + c_4 t^4 + c_5 t^5 + c_6 t^6 + c_7 t^7. \tag{21}$$

Substituting this solution into Eq. (3), we conclude (see Eq. (5)) that two auxiliary polynomials $\overline{S}_6(t)$ and $\overline{S}_7(t)$ with the leading terms t^6 and t^7 are required:

$$\overline{S}_6(t) = \frac{d^2\overline{T}_8(t)}{dt^2},\ \overline{S}_7(t) = \frac{d^2\overline{T}_9(t)}{dt^2},$$

$$\overline{T}_8(t) = T_8\left(\frac{t}{2} - 1\right),\ \overline{T}_9(t) = T_9\left(\frac{t}{2} - 1\right),$$

$$T_8(\tau) = 128\tau^8 - 256\tau^6 + 160\tau^4 + 32\tau^2 - 1,$$

$$T_9(\tau) = 256\tau^9 - 576\tau^7 + 432\tau^5 - 120\tau^3 + 9\tau.$$

In view of Eqs. (19) for the initial conditions, we obtain the following relations:

$$x''(t) + tx'(t) + 2x(t) \equiv \tau_6\overline{S}_6(t) + \tau_7\overline{S}_7(t),$$

$$x(0) - \tau_6\overline{T}_8(0) - \tau_7\overline{T}_9(0) = 0,$$

$$x'(0) - \tau_6\overline{T}_8'(0) - \tau_7\overline{T}_9'(0) = 1.$$

We obtain the following solution of the corresponding SLAE with respect to unknown coefficients:

$$\begin{gathered} c_0 \approx 0.00234716,\ c_1 \approx 0.92262700, \\ c_2 \approx 0.41914500,\ c_3 \approx -1.45266000, \\ c_4 \approx 0.78428300,\ c_5 \approx -0.20136600, \\ c_6 \approx 0.02406430,\ c_7 \approx -0.00106550. \end{gathered} \tag{22}$$

Figs. 3 and 4 illustrate the accuracy of the approximate solution and its first and second-order derivatives. Since there are no visual differences between the graphs of approximate and exact solutions, such graphs are not shown in Fig. 3. The maximum error on the interval $t \in [0.4]$ is 0.0023 for the approximate solution; the error for the first-order derivative is 0.0770; the absolute error for the second-order derivative reaches 0.8400.

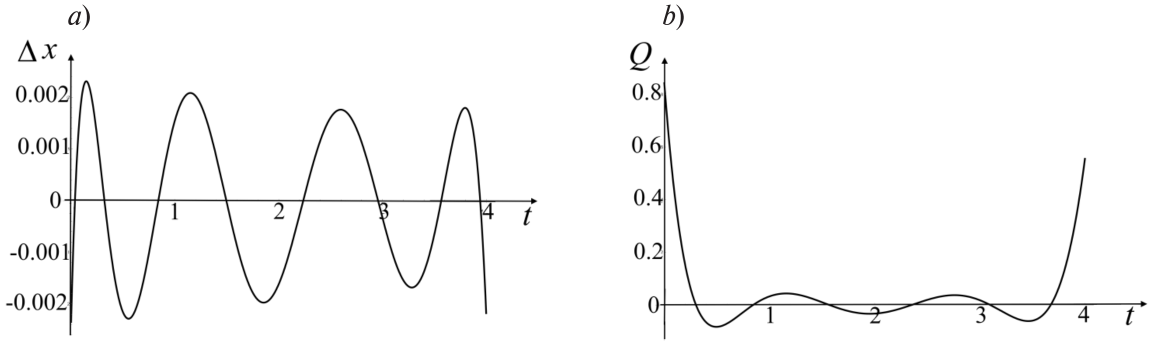

Fig. 3. Characteristics of approximate solution of Eq. (3) obtained by the optimized Tau-method: *a* is the error of this solution, *b* is its differential residual

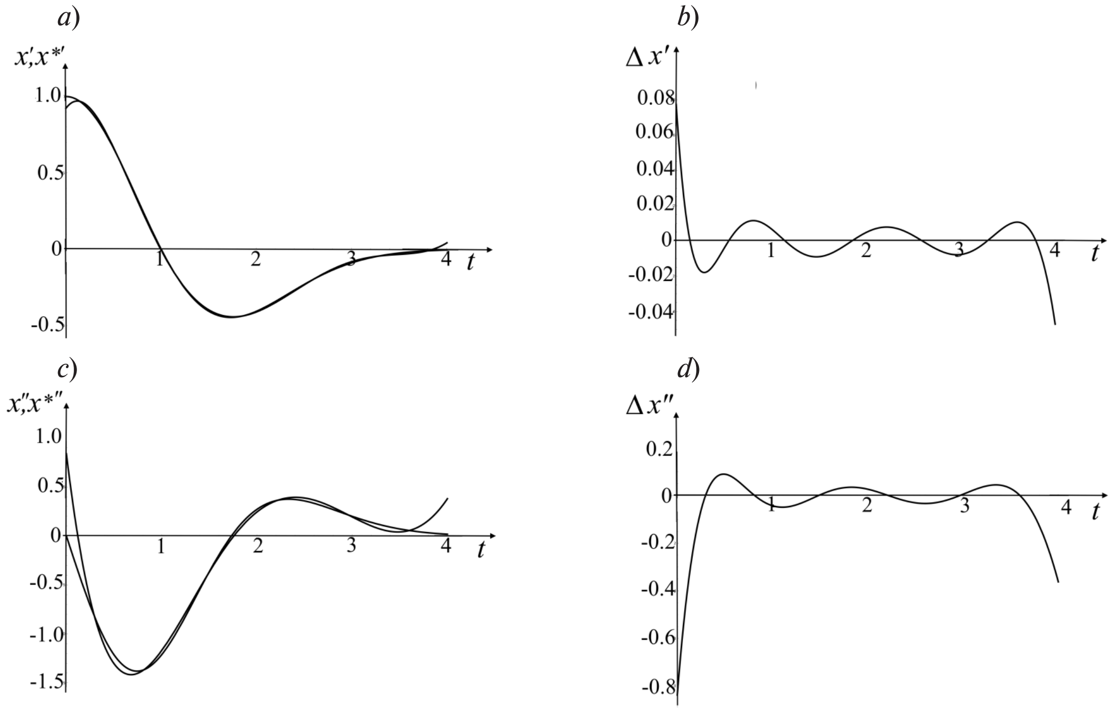

Fig. 4. First (*a*, *b*) and second (*c*, *d*) derivatives of approximate ($x(t)$) and exact ($x^*(t)$) solutions of Eq. (3) (*a*, *c*) and error of derivatives for approximate solution (*b*, *d*). Results were obtained by the optimized Tau-method

Discussion

As mentioned in Remark 2 to Theorem 5, the result may differ from the optimal minimax polynomial if the proposed algorithm uses more than one auxiliary polynomial. To find the true optimal solution, it is necessary to consider a general variational problem, where the free parameters of the approximate solution are used to obtain the least deviating polynomial for the right-hand side of the integral equation.

However, the process of solving such a problem is poorly algorithmized. Substituting the true, least deviating polynomial in the right-hand side of the integral equation by the sum of Chebyshev polynomials makes it possible to reduce the general variational problem to simple algebraic calculations. Even if the error of the approximate solution obtained does not turn out to be the true minimax error, this error is still sufficiently small.

The undoubted advantage of the algorithm under consideration is that it allows to obtain approximate analytical solutions when the coefficients of the equation and/or the initial conditions and/or endpoints of the interval under consideration are algebraic expressions depending on the parameters. This allows to investigate and optimize solutions without numerically solving differential equations for each set of parameters under consideration.

Conclusion

Based on the analysis carried out, we can formulate the following generalizing statements.

1. Minimization of differential residuals of an n-th order LODE or a system of first-order LODEs is not equivalent to minimization of errors of approximate solutions. The polynomial differential residuals in the right-hand sides of the equations used in the Lanczos method should be nth-order derivatives of Chebyshev polynomials and not Chebyshev polynomials themselves.

2. Using approximate initial conditions for approximate solutions gives the researcher more freedom in constructing approximate solutions and ensures greater accuracy. Optimal variations of the initial conditions follow from the analysis of integral residuals, which are linear combinations of scaled Chebyshev polynomials with abstract coefficients calculated subsequently from SLAE of the optimized Tau-method.

3. Derivatives of approximate solutions are not the best approximations to derivatives of exact solutions, even if approximate solutions turn out to be the best approximations to exact solutions. To obtain good approximations for derivatives of exact solutions, it is necessary to transform a linear differential equation with polynomial coefficients into a system of first-order linear differential equations and then apply the Lanczos method to this system. This approach also introduces more free coefficients for varying the approximate solution and, therefore, provides greater accuracy for the best approximate solution.

A separate publication will consider the potential offered by replacing a single differential equation with a system of differential equations in combination with the optimized Tau-method.

The proposed approach is an optimization of the original Lanczos Tau-method for the following reasons.

Firstly, the new method optimizes the error of the approximate solution, whereas the original Tau-method optimizes only the differential residual. However, the error of the approximate solution for high-order differential equations, calculated by multiple iterated integration of the minimum differential discrepancy, may turn out to be very far from the minimum achievable error if the differential residual is not identically zero. The same considerations hold true when some authors use orthogonal polynomials of other types to optimize differential residuals of differential equations.

Secondly, the proposed method introduces a controlled perturbation of the initial conditions. This gives the researcher more freedom to optimize the approximate solution, consequently yielding results with greater accuracy.

Thirdly, error-oriented analysis of integral residuals shows that equations with leading coefficients of polynomials should be considered using adjusted tau algorithms to obtain good accuracy for approximate solutions.

We intend to analyze the special case of the optimized Tau-method, focusing on differential equations with a leading coefficient of the polynomial in a future study.

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