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Geometric Series Bounds for the Local Errors of Taylor Methods for Linear n-th Order ODEs

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1 Introduction

Interval Taylor methods for the validated solution of initial value problems for ODEs were introduced by Moore (1965a, 1965b, 1966). Lohner (1987, 1988, 1992) developed a comprehensive software package of an advanced interval Taylor method, which he applied successfully to many linear and nonlinear problems. But, as Lohner (1988) remarked, the step size of his method is limited by the step size for the explicit Euler method. Lohner (1995), Corliss & Rihm (1996) and Nedialkov (1999) have proposed modified versions of Lohner's algorithm that remove this restriction. However, to the author's knowledge these alternatives have not been extensively tested and have not been implemented in software for general IVPs.

In this paper, a new enclosure method for linear n–th order ODEs is proposed. It is also based on Taylor series expansions, but the foundation of the error bound is completely different from Moore's or Lohner's methods. Its main advantage is that it works with very large step sizes. Recently, (Neher 1999), the method was presented for linear ODEs with polynomial coefficient functions. Here it is extended to linear ODEs with analytic coefficient functions.

We assume that the reader is familiar with interval arithmetic (Moore 1966, Alefeld and Herzberger 1983) and its implementation on a computer (Kulisch and Miranker 1981). Our presentation is concentrated on the analytic foundations of the method rather than on customary interval arithmetic modifications that are necessary when the calculations are performed in floating point arithmetic.

In the next two sections, the model IVP is introduced and an error estimation scheme for a single integration step is developed. After that, we comment on the implementation of the method and on the continuation of the integration of the ODE. In the last section, numerical examples are given.

2 IVP for linear n-th order ODE

For $n \geq 2$, we consider the following normalized initial value problem for a linear ODE with analytic coefficient functions on some interval $[0, r)$:

$$\begin{aligned} y^{(n)} &= \sum_{i=0}^{n-2} p_i(x)\, y^{(i)} + p_{-1}(x), \\ y^{(i)}(0) &= y_{io}, \quad i = 0, \dots, n-1, \end{aligned} \tag{1}$$

where $p_i(x)$, $i = -1, \dots, n-2$ are assumed to be analytic functions with Taylor series

$$p_i(x) \;=\; \sum_{j=0}^{\infty} b_{ij}\, x^j, \quad x \in [0, r). \tag{2}$$

For the numbers b_{ij}, we assume that there are constants $m_i \in \mathbb{N}_0$ and $B_i \geq 0$ such that

$$|b_{ij}| \;\leq\; \frac{B_i}{r^j}, \;\; \text{for } j > m_i, \quad i = -1, \ldots, n-2 \tag{3}$$

(the computation of such bounds will be discussed in Section 5).

Remark: The normalization of the IVP applies for technical reasons, without loss of generality. If the initial values are given at some $x_0 \neq 0$, then let $u(x) := y(x - x_0)$ and reformulate the problem for u. If the differential equation contains also $p_{n-1}(x)\, y^{(n-1)}$ then the transformation $w(x) = y(x) e^{\frac{1}{n}\int p_{n-1}(x)dx}$ yields an ODE of the form (1) for w (cf. Heuser 1989, p. 257).

It is well known (Heuser 1989, p. 260) that the solution of (1) can be written as a power series

$$y(x) \;:=\; \sum_{k=0}^{\infty} a_k\, x^k, \tag{4}$$

and that this series converges at least for all x with $|x| < r$. Inserting the series into (1), we have

$$a_k \;=\; \frac{y_{k0}}{k!} \qquad \text{for } \; k = 0, \ldots, n-1, \tag{5}$$

$$a_{k+n} \;=\; \sum_{i=0}^{n-2} \sum_{j=0}^{k} \frac{P(k-j, i)\, b_{ij}}{P(k, n)}\, a_{k+i-j} \;+\; \frac{b_{-1,k}}{P(k, n)} \quad \text{for } \; k = 0, 1, \ldots, \tag{6}$$

where

$$P(k, i) \;:=\; (k+1) \cdots (k+i), \quad P(k, 0) \;:=\; 1 \quad \text{ for } \; i \in \mathbb{N}, k \in \mathbb{N}_0.$$

3 Error estimation for the IVP

We use (4) to construct lower and upper bounds of $y(h)$ for some $h \in [0, r)$. A pair of such bounds is called an *enclosure* of $y(h)$.

First, we compute finitely many, say κ, coefficients a_k from (5) and (6) and then use the truncated series

$$s(\kappa) \;:=\; \sum_{k=0}^{\kappa-1} a_k\, h^k \tag{7}$$

as an approximation to $y(h)$. The approximation error $y(h) - s(\kappa)$ is then the truncation error given by the infinite series

$$t(\kappa) \;:=\; \sum_{k=\kappa}^{\infty} a_k\, h^k.$$

Our goal is to bound $t(\kappa)$ by a geometric series. As a prerequisite, we recall an elementary summation formula. For $i \in \mathbb{N}_0$, the proof is with induction with respect to k.

Lemma 1 *For all* $i, k \in \mathbb{N}_0$*:* $\quad \displaystyle\sum_{j=0}^{k} P(j,i) = \frac{P(k,i+1)}{i+1}$.

Now suppose that (3) holds. Then we can deduce the following theorem:

Theorem 1 *The sequence* $\{a_k r^k\}_{k=0}^{\infty}$ *with* a_k *from (5) and (6) is bounded.*

Proof: Let $m := \max_{i=-1}^{n-2} m_i$. Then for $k > m$,

$$
\begin{aligned}
|a_{k+n}\, r^{k+n}| \overset{(6)}{\leq} & \sum_{i=0}^{n-2}\sum_{j=0}^{m_i} \frac{r^{n-i}\, P(k-j,i)\ |b_{ij}|\, r^j}{P(k,n)}\ |a_{k+i-j}|\ r^{k+i-j} \\
& + \sum_{i=0}^{n-2}\ \sum_{j=m_i+1}^{k} \frac{r^{n-i}\, P(k-j,i)\ |b_{ij}|\, r^j}{P(k,n)}\ |a_{k+i-j}|\ r^{k+i-j} + \frac{|b_{-1,k}|\ r^{k+n}}{P(k,n)} \\
\overset{(3)}{\leq} & \max_{\nu=k-m}^{k+n-2} |a_\nu\, r^\nu| \sum_{i=0}^{n-2}\sum_{j=0}^{m_i} \frac{r^{n-i+j}\ P(k-j,i)\ |b_{ij}|}{P(k,n)} \\
& + \max_{\nu=0}^{k+n-2} |a_\nu\, r^\nu| \sum_{i=0}^{n-2} \frac{B_i\, r^{n-i}}{P(k,n)} \sum_{j=m_i+1}^{k} P(k-j,i) + \frac{B_{-1}\, r^n}{P(k,n)} \\
\overset{\text{Lemma 1}}{=} & \max_{\nu=k-m}^{k+n-2} |a_\nu\, r^\nu| \sum_{i=0}^{n-2}\sum_{j=0}^{m_i} \frac{r^{n-i+j}\ P(k-j,i)\ |b_{ij}|}{P(k,n)} \\
& + \max_{\nu=0}^{k+n-2} |a_\nu\, r^\nu| \sum_{i=0}^{n-2} \frac{B_i\, r^{n-i}\, P(k-m_i-1,i+1)}{(i+1)\, P(k,n)} + \frac{B_{-1}\, r^n}{P(k,n)} \\
\leq & \max_{\nu=0}^{k+n-1} |a_\nu\, r^\nu| \Bigg\{ \underbrace{\frac{\max_{\nu=k-m}^{k+n-1} |a_\nu\, r^\nu|}{\max_{\nu=0}^{k+n-1} |a_\nu\, r^\nu|}}_{\leq 1} \sum_{i=0}^{n-2}\sum_{j=0}^{m_i} \underbrace{\frac{r^{n-i+j}\ P(k-j,i)\ |b_{ij}|}{P(k,n)}}_{\searrow 0\ (k\to\infty)} \\
& + \sum_{i=0}^{n-2} \underbrace{\frac{B_i\, r^{n-i}\, P(k-m_i-1,i+1)}{(i+1)\, P(k,n)}}_{\searrow 0\ (k\to\infty)} + \underbrace{\frac{B_{-1}\, r^n}{P(k,n)}}_{\searrow 0} \cdot \underbrace{\frac{1}{\max_{\nu=0}^{k+n-1} |a_\nu\, r^\nu|}}_{\text{nonincreasing}} \Bigg\}.
\end{aligned}
$$

(In the last inequality, the upper indexes on the maxima have been increased on purpose.)

Since the (finitely many) summands within the brackets tend to zero for $k \to \infty$, there is a number κ so that the *recess condition*

$$\frac{\max_{\nu=k-m}^{k+n-1} |a_\nu\, r^\nu|}{\max_{\nu=0}^{k+n-1} |a_\nu\, r^\nu|} \sum_{i=0}^{n-2} \sum_{j=0}^{m_i} \frac{r^{n-i+j}\, P(k-j,i)\, |b_{ij}|}{P(k,n)} + \sum_{i=0}^{n-2} \frac{B_i\, r^{n-i}\, P(k-m_i-1,i+1)}{(i+1)\, P(k,n)} + \frac{B_{-1}\, r^n}{P(k,n) \max_{\nu=0}^{k+n-1} |a_\nu\, r^\nu|} \leq 1 \tag{8}$$

holds for all $k \geq \kappa$. Hence,

$$|a_{\kappa+n}\, r^{\kappa+n}| \leq \max_{\nu=0}^{\kappa+n-1} |a_\nu\, r^\nu|\,,$$

and, by induction,

$$|a_k\, r^k| \leq A := \max_{\nu=0}^{\kappa+n-1} |a_\nu\, r^\nu| \quad \text{for all} \quad k \in \mathbf{N}_0\,. \tag{9}$$

□

For a given IVP (1), the smallest number κ that fulfills (8) and the number A defined in (9) depend on r. This dependency can be the basis of a step size and order control strategy in practical computations, as will be outlined in Section 5.

As a direct consequence of Theorem 1, $t(\kappa)$ is bounded by a geometric series for $0 \leq h < r$:

Corollary 1 *Under the above assumptions, for $h = \omega r$, $0 \leq \omega < 1$, and all $k \geq 0$,*

$$|\, y(h) - \sum_{\nu=0}^{k-1} a_\nu\, h^\nu \,| \leq \sum_{\nu=k}^{\infty} |a_\nu\, r^\nu|\, \omega^\nu \leq A \sum_{\nu=k}^{\infty} \omega^\nu = \frac{A\,\omega^k}{1-\omega},$$

where A is defined by (9).

Continuous enclosures of the solution, that is lower and upper function bounds for $y(x)$ on $[0, r)$, follow immediately:

Corollary 2 *Under the above assumptions, for $x \in [0, r)$ and all $k \geq 0$,*

$$|\, y(x) - \sum_{\nu=0}^{k-1} a_\nu\, x^\nu \,| \leq A \sum_{\nu=k}^{\infty} \left(\frac{x}{r}\right)^\nu = A \cdot \frac{\left(\frac{x}{r}\right)^k}{1-\frac{x}{r}}.$$

4 Continuation of the integration

So far, we have only described one step of the integration of the given IVP. When the integration domain is split into subintervals, then initial values for the first $n-1$ derivatives are required on subsequent integration intervals. Also, since all intermediate errors must be enclosed in the course of computation, instead of real initial values one has to deal with interval initial values that include the set of all possible real initial values.

4.1 Enclosures of derivatives

Enclosures for derivatives at $x = h$ are gained by an estimation of the truncation error similar to the estimation according to Corollary 1. From (4),

$$y^{(i)}(h) \;=\; \sum_{\nu=i}^{\infty} P(\nu-i,i)\, a_\nu\, h^{\nu-i}.$$

If $A = \max_{\nu=0}^{\infty} |a_\nu r^\nu|$ and if κ and q are such that (12) and (13) hold, then for $k \geq \kappa$,

$$|y^{(i)}(h) - \sum_{\nu=i}^{k-1} P(\nu-i,i)\, a_\nu\, h^{\nu-i}| \;\leq\; \sum_{\nu=k}^{\infty} P(\nu-i,i)\; |a_\nu|\; r^\nu\, r^{-i} \omega^{\nu-i}$$

$$\leq\; \frac{qA}{r^i} \sum_{\nu=k}^{\infty} P(\nu-i,i)\, \omega^{\nu-i} \;=\; \frac{qA}{r^i}\frac{d^i}{d\omega^i} \sum_{\nu=k}^{\infty} \omega^\nu \;=\; \frac{qA}{r^i}\frac{d^i}{d\omega^i}\frac{\omega^k}{1-\omega}\;.$$

We conclude that error bounds for derivatives of the solution y of (1) follow immediately from error bounds for y.

4.2 Interval initial values

Let us assume that the integration domain $[0, x_J]$ is split into J subintervals $I_j = [x_{j-1}, x_j]$, $j = 1, \ldots, J$, and that in each subinterval I_j, $j \geq 1$, interval initial values appear. Real initial value problems are then used to compute tight enclosures of y. In the case of a homogeneous differential equation, n initial value problems

$$u_\nu^{(n)} \;=\; \sum_{i=0}^{n-2} p_i(x)\, u_\nu^{(i)}, \quad x \in I_j,$$
$$u_\nu^{(\mu)}(x_{j-1}) \;=\; \delta_{\mu\nu}, \quad \mu,\nu = 0,1,\ldots,n-1,$$

replace one interval initial value problem. If interval matrices $[A_j] = ([a_{\mu\nu}^j])$ are built of intervals $[a_{\mu\nu}^j] \ni u_\nu^{(\mu)}(x_j)$ for $j = 1, \ldots, J$, then $y(x_J)$ is contained in the first component of the matrices–vector product

$$[A_J]C_J\Big(C_J^{-1}[A_{J-1}]C_{J-1}\Big(\cdots\Big(C_3^{-1}[A_2]C_2\Big(C_2^{-1}[A_1]\begin{pmatrix} y(0)\\ \vdots \\ y^{(n-1)}(0)\end{pmatrix}\Big)\cdots\Big), \qquad (10)$$

where the C_j are arbitrary nonsingular matrices. Using $n+1$ IVPs on each subinterval, a similar representation can be derived for nonhomogeneous ODEs.

The matrices C_j are used to rule out the wrapping effect that appears when intermediate results of successive matrix-vector multiplications are stored in interval vectors. Lohner (1987, 1988, 1992) discussed several choices for the matrices C_j.

5 Practical calculation of the enclosure

By Corollary 1, the enclosure of $y(h)$ is built from the Taylor polynomial approximate solution $s(\kappa)$ in (7) and a geometric series error bound. For the construction of $s(\kappa)$, only finitely many Taylor coefficients b_{ij} in (2) are needed. They are obtained by automatic differentiation (Rall 1981) of the functions p_i. The numbers a_k in (7) are then calculated recursively from (5) and (6).

The geometric series bound relies on the bounds B_i in (3) and on a number κ such that (8) holds for all $k \geq \kappa$. The calculation of these quantities will be described in two subsections. The number A then follows from (9).

5.1 Estimates for Taylor coefficients of analytic functions

A well known bound for Taylor coefficients of analytic functions is Cauchy's estimate (Conway 1973, p. 73). For an analytic function

$$p(z) \;=\; \sum_{j=0}^{\infty} b_j z^j, \qquad |z| \leq r,$$

it holds that

$$|b_j| \;\leq\; \frac{\max_{|z|=r} |p(z)|}{r^j}, \qquad j \in \mathbb{N}.$$

Now let $T_{m_i}(z;p_i)$ denote the Taylor polynomial of order m_i for p_i in (1). Then we can use

$$B_i \;:=\; \max_{|z|=r} |p_i(z) - T_{m_i}(z;p_i)|\,, \qquad i=-1,\ldots,n-2 \qquad (11)$$

in (3). The practical computation of B_i has thus become the problem of determining the range of a complex function.

For many compositions of complex standard functions, the real and the imaginary parts can be expressed by compositions of real standard functions. Braune and Krämer (1987) used these decompositions for the construction of high–accuracy complex interval standard functions that are easily implemented in modern programming languages, and that yield tight range bounds.

5.2 Determination of κ

If κ is a given integer, then we can check the recess condition (8) for $k = \kappa$. However, the fulfillment of (8) for $k = \kappa$ does not imply that (8) holds for all $k \geq \kappa$, because the left of (8) is not monotonically decreasing with k in general. Monotonicity only holds for some of the terms and for sufficiently large k (the proof of Lemma 2 follows from straightforward calculations):

Lemma 2 *For $k \geq n(m+1)$, $\dfrac{P(k-j,i)}{P(k,n)}$ and $\dfrac{P(k-m_i-1,i+1)}{P(k,n)}$ are monotonically decreasing with k.*

$\dfrac{\max_{\nu=k-m}^{k+n-1} |a_\nu\, r^\nu|}{\max_{\nu=0}^{k+n-1} |a_\nu\, r^\nu|}$ is not necessarily monotonic with k, not even for large k. Hence, we modify the recess condition slightly, to obtain an enclosure criterion that is verifiable by simple practical calculations. Suppose that for some $k \geq n(m+1)$ and some q, $0 < q < 1$, it holds that

$$\frac{\max\limits_{\nu=k-m}^{k+n-1} |a_\nu r^\nu|}{\max\limits_{\nu=0}^{k+n-1} |a_\nu r^\nu|} \;\leq\; q \tag{12}$$

and that

$$\begin{aligned} & q \cdot \sum_{i=0}^{n-2} \sum_{j=0}^{m_i} \frac{r^{n-i+j}\, P(k-j,i)\, |b_{ij}|}{P(k,n)} \\ & + \sum_{i=0}^{n-1} \frac{B_i\, r^{n-i}\, P(k-m_i-1,i+1)}{(i+1)\, P(k,n)} \;+\; \frac{B_{-1}\, r^n}{P(k,n)} \;\leq\; q. \end{aligned} \tag{13}$$

Then

$$|a_{k+n} r^{k+n}| \;\leq\; q \cdot \max_{\nu=0}^{k+n-1} |a_\nu r^\nu|\,,$$

so that

$$|a_{k+j} r^{k+j}| \;\leq\; q \cdot \max_{\nu=0}^{k+n-1} |a_\nu r^\nu| \quad \text{for all } j \geq n.$$

Due to Lemma 2, the fulfillment of (12) and (13) for $k = \kappa \geq n(m+1)$ is a sufficient condition that (12) and (13) also hold for all $k > \kappa$. Instead of A we can then use qA in Corollary 1 or Corollary 2, to obtain pointwise or continuous enclosures of the solution of the given IVP (1).

5.3 Step size and order control strategy

In many numerical examples, the following step size and order control strategy has been found to be effective: If the interval of integration is given by $[0, x_J]$, then start the enclosure algorithm with $h = x_J$. Choose $\omega \in (0,1)$ (often, $\omega \in (0.5, 0.9)$ proved to be a good choice) and let $r := \frac{h}{\omega}$. Compute the numbers B_i from (11), provided that the functions p_i are analytic for $|z| \leq r$. Check the modified recess condition (13) for $q = 1$ and a suitable value of $k = \kappa$ (the approximate order of the method). If (13) is fulfilled, then compute $s(\kappa)$ and enclose $t(\kappa)$ according to Corollary 1. Increase κ until $t(\kappa)$ becomes small enough for an accurate enclosure of $y(h)$. If any of the above steps failed, then bisect the integration domain and apply the same procedure recursively to both subintervals.

6 Numerical examples

We have implemented our method in a computer program written in PASCAL–XSC (Klatte et al. 1992), a PASCAL extension with a machine interval arithmetic. In such an arithmetic, all of the above calculations can be performed virtually unchanged, by replacing all operations between real numbers by the corresponding operations between machine intervals, with the automatic enclosure of all roundoff errors in the result of any computation.

The program includes a multiple precision interval staggered correction arithmetic (Stetter 1984), to handle the cancellations that occur when the calculations are performed in floating arithmetic. The complete code of the program is available via Internet at

`http//www.uni-karlsruhe.de/~Markus.Neher/livptayp.html`

Example 1: $y'' = \alpha e^x y + e^{-x} - \alpha,\ y(0) = 1,\ y'(0) = -1.$

The exact solution of this problem is $y(x) = e^{-x}$. The IVP gets numerically unstable when α is increasing. In Table 1 we show the computed enclosures $[y(h)]$ for several values of α and for the largest values of h that could be reached with one single integration step (for $\omega = 0.82$ and $\kappa \leq 300$). The computation times (in seconds) were obtained on a PC with a Pentium II processor with 266 MHz.

In the last column the maximum integration domains that were reached with Lohner's program AWA (that runs with single precision) are given. Long before the integration with AWA aborted, the enclosures had already become inaccurate.

Table 1. Integrations for different values of α.

α	x	κ	$[y](x)$	Time	$x_{\max}$ with AWA
100	3.25	288	$3.877\,420\,783\,172\,20^{3}_{0}$E-02	54	2.231
1000	2	261	$1.353\,352\,832\,366\,12^{8}_{6}$E-01	47	0.981
10000	1	279	$3.678\,794\,411\,714\,^{588}_{354}$E-01	47	0.356

Example 2: Computation of eigenvalues of

$$\begin{array}{rcl} -u'' + \cos(2x)\,u & = & \lambda u \\ u(0) = u(\pi) & = & 0. \end{array} \tag{14}$$

A real number λ is called an eigenvalue of the boundary value problem (14) if there is a nontrivial solution $u(x)$ of (14). Following the well–known Sturm–Liouville theory, we compute eigenvalues of (14) with a shooting method with shooting parameter λ, using the initial value problem

$$\begin{array}{rcl} y'' & = & (\cos x - \lambda)\,y \\ y(0) & = & 0,\ y'(0) = 1. \end{array} \tag{15}$$

If $y(\pi;\lambda) = 0$ then λ is an eigenvalue of (14). The index of the eigenvalue is given by the number of zeros of $y(\cdot;\lambda)$ in the interval $(0,\pi)$. Due to the symmetry of the differential equation and the boundary conditions, eigenvalues can also be computed by testing $y(\frac{\pi}{2}) = 0$ (for eigenvalues with even indexes) or $y'(\frac{\pi}{2}) = 0$ (for eigenvalues with odd indexes). Eigenvalue bounds for specific eigenvalues are computed by solving (15) for different values of λ and $x \in [0,\pi]$, and by determining the number $N(\lambda)$ of zeros of the respective solutions $y(\cdot;\lambda)$ within $(0,\pi)$.

The latter task involves validated rootfinding. The zeros are all simple and isolated. Uniqueness of a root in a given interval $X = [x_1, x_2] \subset [0,\pi]$ can be proved with a continuous enclosure of the derivative of $y(\cdot;\lambda)$ (Neher 1992). Let U be an interval such that $y'(x,\lambda) \in U$ for all $x \in X$, then $y(x,\lambda)$ has a unique zero in X if $y(x_1,\lambda)\cdot y(x_2,\lambda) < 0$ and $0 \notin U$ holds.

Table 2. Integrations of (15) for different values of λ.

λ	$N(\lambda)$	$[y(\frac{\pi}{2})]$
16.008 310 459 709 47	3	$-3.87^{4}_{5}\mathrm{E}-16$
16.008 310 459 709 48	4	$1.36^{6}_{5}\mathrm{E}-16$
λ	$N(\lambda)$	$[y'(\frac{\pi}{2})]$
121.001 041 672 579 0	10	$-1.00^{7}_{8}\mathrm{E}-16$
121.001 041 672 579 1	11	$^{7.27}_{6.79}\mathrm{E}-15$

In Table 2, the enclosures of $y(\frac{\pi}{2};\lambda)$ from (15) are listed for four different values of λ. They were computed with only one integration step. From these enclosures, the eigenvalues λ_4 and λ_{10} of (14) are determined with 16 decimal digits of accuracy:

$$\lambda_4 \in 16.008\,310\,459\,709\,4^{8}_{7},$$
$$\lambda_{10} \in 121.001\,041\,672\,579\,^{1}_{0}.$$

Conclusion

We have presented a new enclosure method for linear n-th order ODEs with analytic coefficients. Our numerical examples demonstrate that the method can be successfully implemented on a computer, and that it works with very large step sizes.

Future work will concentrate on the utilization of the method to nonlinear ODEs.

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