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SOME RECENT ADVANCES IN VALIDATED METHODS FOR IVP'S FOR ODE'S*

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We present an overview of interval Taylor series (ITS) methods for IVPs for ODEs and discuss some recent advances in the theory of validated methods for IVPs for ODEs, such as, an interval Hermite-Obreschkoff (IHO) scheme, the stability of ITS and IHO methods, and a new perspective on the wrapping effect.

1. Introduction. We consider the set of autonomous IVPs

$$y'(t) = f(y) \tag{1}$$

$$y(t_0) \in [y_0], \tag{2}$$

where $t \in [t_0, t_m]$ for some $t_m > t_0$. Here t_0 and $t_m \in \mathbf{R}$, $f \in C^{k-1}(\mathcal{D})$, $\mathcal{D} \subseteq \mathbf{R}^n$ is open, $f : \mathcal{D} \to \mathbf{R}^n$, and $[y_0] \subseteq \mathcal{D}$.

We consider a grid $t_0 < t_1 < \cdots < t_m$ and denote the stepsize from t_{j-1} to t_j by $h_{j-1} = t_j - t_{j-1}$. We denote the solution of (1) with an initial condition $y(t_{j-1}) = y_{j-1}$ by $y(t; t_{j-1}, y_{j-1})$. For an interval vector $[y_{j-1}]$, we denote by $y(t; t_{j-1}, [y_{j-1}])$ the set of solutions $\{\, y(t; t_{j-1}, y_{j-1}) \mid y_{j-1} \in [y_{j-1}] \,\}$.

Our goal is to compute interval vectors $[y_j]$, $j = 1, 2, \ldots, m$, that are guaranteed to contain the solution of (1–2) at $t_1, t_2, \ldots, t_m$. That is,

$$y(t_j; t_0, [y_0]) \subseteq [y_j], \quad \text{for } j = 1, 2, \ldots, m.$$

Usually, validated methods for IVPs for ODEs are one-step methods, where each step consists of two phases [7], [9]:

Algorithm I: validate existence and uniqueness of the solution with some stepsize, and
Algorithm II: compute a tight enclosure for the solution.

We present an overview of interval Taylor series (ITS) methods for IVPs for ODEs and discuss some recent advances in the area of validated ODE solving. In particular, we discuss

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- an interval Hermite-Obreschkoff (IHO) scheme for computing tight enclosures on the solution [5];
- instability in interval methods for IVPs for ODEs due to the associated formula for the truncation error [5], which appears to make it difficult to derive effective validated methods for stiff problems; and
- a new perspective on the wrapping effect [6], where we view the problem of reducing the wrapping effect as one of finding a more stable scheme for advancing the solution.

Notation. We use $[\cdot]$ to denote intervals and interval vectors and matrices. For an interval $[a] = [\underline{a}, \bar{a}]$, we define its width, magnitude, and midpoint by

$$\begin{aligned} \mathrm{w}([a]) &= \bar{a} - \underline{a}, \\ |[a]| &= \max\{\,|\underline{a}|, |\bar{a}|\,\}, \text{ and} \\ \mathrm{m}([a]) &= (\underline{a} + \bar{a})/2, \end{aligned}$$

respectively. We define width, magnitude, and midpoint componentwise for interval vectors and matrices.

We define the sequence of functions $f^{[i]}(y)$, $i = 0, 1, 2, \ldots$, by

$$\begin{aligned} f^{[0]}(y) &= y, \\ f^{[i]}(y) &= \frac{1}{i}\left(\frac{\partial f^{[i-1]}}{\partial y} f\right)(y), \quad \text{for } i \geq 1. \end{aligned}$$

For the autonomous IVP (1), $f^{[i]}(y_j) = y^{(i)}(t_j)/i!$. That is, $f^{[i]}(y_j)$ denotes the ith Taylor coefficient of $y(t; t_j, y_j)$ expanded around t_j.

2. Overview of interval methods for IVPs for ODEs.

2.1. Validating existence and uniqueness of the solution. Using the Picard-Lindelöf operator and the Banach fixed-point theorem, one can show that if h_{j-1} and $[\tilde{y}^0_{j-1}] \supseteq [y_{j-1}]$ satisfy

$$[\tilde{y}_{j-1}] = [y_{j-1}] + [0, h_{j-1}]\, f\big([\tilde{y}^0_{j-1}]\big) \subseteq [\tilde{y}^0_{j-1}], \tag{3}$$

then (1) with $y(t_{j-1}) = y_{j-1}$ has a unique solution $y(t; t_{j-1}, y_{j-1}) \in [\tilde{y}_{j-1}]$ for all $t \in [t_{j-1}, t_j]$ and all $y_{j-1} \in [y_{j-1}]$, [1]. A method based on (3) can be implemented easily, but a serious disadvantage of this approach is that it often restricts the stepsize Algorithm II could take.

If we use more Taylor series terms in the sum in (3), we obtain a high-order Taylor series enclosure method [8]. In the latter, we determine h_{j-1} and $[\tilde{y}_{j-1}]$ such that

$$\sum_{i=0}^{k-1} (t - t_{j-1})^i f^{[i]}(y_{j-1}) + (t - t_{j-1})^k f^{[k]}([\tilde{y}_{j-1}]) \subseteq [\tilde{y}_{j-1}] \tag{4}$$

holds for all $t \in [t_{j-1}, t_{j-1} + h_{j-1}]$ and all $y_{j-1} \in [y_{j-1}]$. Then (1) with $y(t_{j-1}) = y_{j-1}$ has a unique solution $y(t; t_{j-1}, y_{j-1}) \in [\tilde{y}_{j-1}]$ for all $t \in [t_{j-1}, t_j]$ and all $y_{j-1} \in [y_{j-1}]$.

In [8], we show that, for many problems, an interval method based on (4) is more efficient than one based on (3).

2.2. Computing a tight enclosure of the solution. Consider the Taylor series expansion

$$y_j = y_{j-1} + \sum_{i=1}^{k-1} h_{j-1}^i f^{[i]}(y_{j-1}) + h_{j-1}^k f^{[k]}(y; t_{j-1}, t_j), \tag{5}$$

where $y_{j-1} \in [y_{j-1}]$, and $f^{[k]}(y; t_{j-1}, t_j)$ denotes $f^{[k]}$ with its lth component ($l = 1, 2, \dots, n$) evaluated at $y(\xi_{j-1,l})$ for some $\xi_{j-1,l} \in [t_{j-1}, t_j]$. Let

$$[S_{j-1}] = I + \sum_{i=1}^{k-1} h_{j-1}^i \, J\left(f^{[i]}; [y_{j-1})\right] \quad \text{and} \quad [z_j] = h_{j-1}^k f^{[k]}([\tilde{y}_{j-1}]), \tag{6}$$

where $J\left(f^{[i]}; [y_{j-1})\right]$ is the Jacobian of $f^{[i]}$ evaluated at $[y_j]$, and $[z_j]$ is an enclosure of the local error.

If we apply the mean-value theorem to $f^{[i]}$ in (5) and use (6), we obtain that, for any $\hat{y}_{j-1} \in [y_{j-1}]$,

$$y(t_j; t_0, [y_0]) \in [y_j] = \hat{y}_{j-1} + \sum_{i=0}^{k-1} h_{j-1}^i f^{[i]}(\hat{y}_{j-1}) + [z_j] + [S_{j-1}]([y_{j-1}] - \hat{y}_{j-1}). \tag{7}$$

We can compute enclosures on the solution of (1–2) with (7). However, this approach frequently works poorly, because the interval vector $[S_{j-1}]([y_{j-1}]-\hat{y}_{j-1})$ may significantly overestimate the set

$$\{\, S_{j-1}(y_{j-1} - \hat{y}_{j-1}) \mid S_{j-1} \in [S_{j-1}],\ y_{j-1} \in [y_{j-1}] \,\}.$$

Such overestimations normallly accumulate as the integration proceeds. As a result, we have the wrapping effect [4].

Lohner's QR-factorization method. Lohner's QR-factorization method [3] is one of the most successful, general-purpose methods for reducing the wrapping effect. In this method, we compute

$$[y_j] = \hat{y}_{j-1} + \sum_{i=1}^{k-1} h_{j-1}^i f^{[i]}(\hat{y}_{j-1}) + [z_j] + \big([S_{j-1}]\, A_{j-1}\big)[r_{j-1}],$$

instead of (7), and propagate

$$[r_j] = \big(A_j^{-1}([S_{j-1}]\, A_{j-1})\big)[r_{j-1}] + A_j^{-1}\big([z_j] - \mathrm{m}([z_j])\big),$$

where

$$\begin{aligned} \hat{y}_0 &= \mathrm{m}([y_0]),\ \ [r_0] = [y_0] - \hat{y}_0, \quad \text{and} \\ \hat{y}_j &= \hat{y}_{j-1} + \sum_{i=1}^{k-1} h_{j-1}^i f^{[i]}(\hat{y}_{j-1}) + \mathrm{m}([z_j]) \quad (j \geq 1). \end{aligned}$$

Here, $A_0 = I$, and for $j \geq 1$, A_j is the orthogonal matrix from the QR factorization of $\mathrm{m}([S_{j-1}]A_{j-1})$. One explanation why this method is successful at reducing the wrapping effect is that we enclose the solution on each step in a moving orthogonal coordinate system that "matches" the solution set [3].

3. An interval Hermite-Obreschkoff method. Recently, we developed an interval Hermite-Obreschkoff (IHO) method [5], which is based on the formula

$$\begin{aligned} \sum_{i=0}^{q}(-1)^i c_i^{q,p} h_{j-1}^i f^{[i]}(y_j) &= \sum_{i=0}^{p} c_i^{p,q} h_{j-1}^i f^{[i]}(y_{j-1}) \\ &+ (-1)^q \frac{q!p!}{(p+q)!} h_{j-1}^{p+q+1} f^{[k]}(y; t_{j-1}, t_j), \end{aligned} \tag{8}$$

where $c_i^{q,p} = q!(q+p-i)!/((p+q)!\,(q-i)!)$, ($q, p$, and $i \geq 0$), $y_{j-1} = y(t_{j-1}; t_0, y_0)$, and $y_j = y(t_j; t_0, y_0)$.

The method we propose in [5] consists of a predictor phase and a corrector phase. The predictor computes an enclosure $[y_j^0]$ of the solution at t_j, and using this enclosure, the corrector computes a tighter enclosure $[y_j] \subseteq [y_j^0]$ at t_j. If $q > 0$, (8) is an implicit scheme. The corrector applies a Newton-like step to tighten $[y_j^0]$.

We have shown in [5] that for the same order and stepsize, our IHO method has smaller local error, better stability, and requires fewer Jacobian evaluations than an ITS method. The extra cost of the Newton step is one matrix inversion and a few matrix multiplications.

4. Instability from the formula for the truncation error. We considered in [5] the ITS and IHO methods when applied with a constant stepsize h and order k to the test problem

$$y' = \lambda y, \quad y(0) = y_0, \tag{9}$$

where λ and $y_0 \in \mathbf{R}$, and $\lambda < 0$.

Let $T_r(z) = \sum_{i=0}^{r} z^i/i!$. We showed in [5] that, if

$$|T_{k-1}(\lambda h)| + \frac{|\lambda h|^k}{k!} > 1, \tag{10}$$

the ITS method is *asymptotically unstable*, in the sense that $\lim_{j\to\infty} \mathrm{w}([y_j]) = \infty$. Therefore, we have restrictions on the stepsize not only from the function $T_{k-1}(\lambda h)$, as in point methods for IVPs for ODEs, but also from the factor $|\lambda h|^k/k!$ in the remainder term.

Let

$$\begin{aligned} R_{p,q}(z) &= \frac{\sum_{i=0}^{p} c_i^{p,q} \frac{z^i}{i!}}{\sum_{i=0}^{q} c_i^{q,p} \frac{(-z)^i}{i!}}, \quad Q_{p,q}(z) = \sum_{i=0}^{q} c_i^{q,p} \frac{(-z)^i}{i!}, \quad \text{and} \\ \gamma_{p,q} &= \frac{q!p!}{(p+q)!}. \end{aligned}$$

We showed in [5] that, when applied to (9), the IHO method is asymptotically unstable in the sense that $\lim_{j\to\infty} \mathrm{w}([y_j]) = \infty$ for h satisfying

$$|R_{p,q}(\lambda h)| + \frac{\gamma_{p,q}}{|Q_{p,q}(\lambda h)|}\frac{|\lambda h|^k}{k!} > 1. \tag{11}$$

Roughly speaking, the stepsize in the ITS method is restricted by both

$$|T_{k-1}(\lambda h)| \quad \text{and} \quad \frac{|\lambda h|^k}{k!},$$

while in the IHO method, the stepsize is limited mainly by

$$\frac{\gamma_{p,q}}{|Q_{p,q}(\lambda h)|}\frac{|\lambda h|^k}{k!}.$$

In the latter case, $\gamma_{p,q}/Q_{p,q}(\lambda h)$ is usually much smaller than one; thus, the stepsize limit for the IHO method is usually much larger than for the ITS method.

An important point to note here is that an interval version of a standard numerical method, such as the Hermite-Obreschkoff formula (8), that is suitable for stiff problems may still have a restriction on the stepsize. To obtain an interval method without a stepsize restriction, we must find a stable formula not only for the propagated error, but also for the associated truncation error.

5. A new perspective on the wrapping effect. The problem of reducing the wrapping effect has usually been studied from a geometric perspective as finding an enclosing set that introduces as little overestimation of the enclosed set as possible. For example, parallelepipeds, ellipsoids, convex polygons, and zonotopes have been employed to reduce the wrapping effect (see [6] and the references there in).

In [6], we linked the wrapping effect to the stability of an ITS method for IVPs for ODEs and interpreted the problem of reducing the wrapping effect as one of finding a more stable scheme for advancing the solution. This allowed us to study the stability of several ITS methods (and thereby the wrapping effect) by employing eigenvalue techniques, which have proven so useful in studying the stability of point methods. Here, we outline our main results.

Consider the IVP

$$y' = By, \quad y(0) = y_0, \tag{12}$$

where $B \in \mathbf{R}^{n\times n}$ and $n \geq 2$, and let $T = T_{k-1}(hB)$.

When applied with a constant stepsize and order to (12), Lohner's QR-factorization scheme reduces to

$$[y_j] = T\hat{y}_{j-1} + \big(Q_jR_j\big)[r_{j-1}] + [z_j] \tag{13}$$

$$[r_j] = R_j[r_{j-1}] + Q_j^T\big([z_j] - s_j\big), \tag{14}$$

where

$$Q_0 = I \quad \text{and} \quad TQ_{j-1} = Q_jR_j, \quad \text{for } j \geq 1. \tag{15}$$

The interval vector $[r_j]$ in (14) can be interpreted as an enclosure of the global error that is propagated to the next step. Since

$$\mathrm{w}([r_j]) = |R_j|\mathrm{w}([r_{j-1}]) + |Q_j^T|\mathrm{w}([z_j])$$

(see [6]), we can consider $|R_j|$ as the matrix for propagating the global error in the QR method. A key observation in [6] is that (15) is the *simultaneous iteration* for computing the eigenvalues of T (see for example [10]). This iteration is closely related to Francis' QR algorithm [2] for finding the eigenvalues of T.

Eigenvalues of distinct magnitudes. Assuming that T is nonsingular with eigenvalues of distinct magnitudes, we showed in [6] that

$$\lim_{j\to\infty} \rho(|R_j|) = \rho(R) = \rho(T),$$

and the upper bound for the global error of Lohner's method is not much bigger than the bound for the global error of the corresponding point Taylor series method, for the same stepsize and order.

Eigenvalues of equal magnitude. Assuming that T is nonsingular with at least one complex conjugate pair of eigenvalues and at most two eigenvalues of the same magnitude, we showed in [6] that, as $j \to \infty$,

- if T has a dominant complex conjugate pair of eigenvalues, then $\rho(|R_j|) \geq \rho(T)$, and $\rho(R_j)$ oscillates; and
- if T has a unique real eigenvalue of maximal modulus, then we should generally expect that $\rho(|R_j|) \to \rho(T)$.

The analysis is more difficult in this case, but we illustrated with examples in [6] that the global error in Lohner's method is normally not much bigger than the global error of the corresponding point Taylor series method.

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НЯКОИ СЪВРЕМЕННИ МЕТОДИ С ВЕРИФИКАЦИЯ ЗА РЕШАВАНЕ НА ЗАДАЧА НА КОШИ ЗА ОДУ

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Направен е обзор на методите, използващи интервални Тейлърови развития за решаване задача на Коши за ОДУ. Разгледани са някои съвременни методи с верификация на резултатите за решаване на същата задача, като например един интервален вариант на метода на Ермит-Обрешков. Обсъдена е тяхната устойчивост, както и ефекта на завъртане на интервалната обвивка на множеството от решения.