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Implicit Methods for Enclosing Solutions of ODEs

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Abstract: The paper presents a new enclosure method for initial value problems in systems of ordinary differential equations. Like the common enclosure methods (eg Lohner's algorithm AWA), it is based on Taylor expansion. In contrast to them, however, it is an implicit method. The solution sets of nonlinear inequalities have to be enclosed by a Newton-like algorithm. As the presented examples show, the new method sometimes yields much tighter bounds than any of the common explicit methods.

Key Words: Enclosure methods, Implicit methods, Taylor methods, Initial value problems

1 Introduction

We consider an initial value problem

$$u' = f(u), \quad u(t_0) = u_0, \tag{1}$$

where we only know an interval enclosure $[u_0] \in I\!R^n$ of $u_0 \in I\!R^n$ in general. The function f is assumed to be at least p times continuously differentiable in a domain D with $[u_0] \subseteq D \subseteq I\!R^n$, $p \in I\!N$. There is a unique solution $u(t)$ of (1) in a neighborhood of t_0. Using interval arithmetic, we want to compute verified lower and upper bounds of this solution successively on a grid $\{t_1, t_2, \ldots, t_m\}$ with $t_j > t_{j-1}$ for $j = 1, 2, \ldots, m$.

The most effective methods for handling this problem are based on Taylor expansion. Moore presented the prototype [Moore 65] in 1965. Several modifications [eg Moore 66, Eijgenraam 81, Lohner 88, Rihm 93] have been developed since then. Lohner's algorithm AWA (<u>A</u>nfangs<u>w</u>ert<u>a</u>ufgabe) [Lohner 88] is surely the best-known and most sophisticated variant at present. In the following, we will only consider a single integration step, i.e. the computation of an interval vector $[u]$ satisfying $u(t_1) \in [u]$. This is sufficient to show the fundamental differences between the two types of methods we deal with.

The principle of the above mentioned methods is outlined in Section 2. A new enclosure method (the "implicit method") is introduced in Section 3. The remaining sections deal with particular problems and contain some numerical results. The new method is applied to linear ODE systems in Section 4 and to a nonlinear example in Section 5.

2 Taylor methods

Moore's method and its modifications consist of two major parts. They first generate and verify a coarse enclosure $[U]$ with $u(t) \in [U]$ for all $t \in [t_0, t_1]$ by applying the Banach fixed-point theorem to a particular Picard-Lindelöf operator. Then they evaluate bounds of a Taylor polynomial of the solution at t_1

and enclose the corresponding remainder using the coarse enclosure $[U]$. In the sequel, we assume $[U]$ already to be known. We deal with the second part of the algorithm only. (Verification methods for coarse enclosures are shown in [Corliss and Rihm 96], for instance.)

Let the inclusion $u(t) \in [U]$ hold for all $t \in [t_0, t_1]$. Then we have

$$u(t_1) \in \Psi(u_0; h) + [r] \tag{2}$$

with

$$\Psi(u; h) = u + \sum_{j=1}^{p} \frac{h^j}{j!} f^{(j)}(u), \quad [r] = \frac{h^{p+1}}{(p+1)!} f^{(p+1)}([U]),$$

$$f^{(1)} = f, \quad f^{(j+1)} = \frac{\partial f^{(j)}}{\partial u} f, \quad h = t_1 - t_0.$$

$\Psi(u_0; h)$ is a p-th order Taylor polynomial of the solution. $[r]$ is an enclosure of the corresponding remainder. For a given (real or interval) argument, the Taylor coefficients can be evaluated by means of automatic differentiation [see Moore 66, Rall 81, Lohner 88].

All methods based on Moore's idea use inclusion (2) for verification. If u_0 is known exactly, then we can simply evaluate $\Psi(u_0; h)$. Otherwise, an interval evaluation of Ψ is required. If we replace the variable u in the expression of Ψ by the interval vector $[u_0]$, then we get the enclosure

$$[\tilde{u}] := \Psi([u_0]; h) + [r] = [u_0] + \sum_{j=1}^{p} \frac{h^j}{j!} f^{(j)}([u_0]) + [r].$$

This method, however, is always width-increasing ($w([\tilde{u}]) \geq w([u_0])$) and not suitable for practice. The algorithm AWA and several other methods use a mean-value evaluation [see Rihm 94]:

$$[u] := \Psi(\hat{u}_0; h) + \frac{\partial \Psi}{\partial u}([u_0]; h)([u_0] - \hat{u}_0) + [r] \tag{3}$$

with $\hat{u}_0 \in [u_0]$. Automatic differentiation can again be used to compute the elements of the matrix $\partial\Psi/\partial u$ [see Lohner 88, Rihm 93].

Of course, the AWA code [Lohner 88] is much more complicated. Various techniques are necessary for the reduction of the so-called wrapping effect [Moore 66] which occurs if a whole sequence of integration steps is carried out. However, in a single step, Lohner's method actually yields the enclosure (3).

If $\hat{u}_0$ is the midpoint of $[u_0]$ (denoted by $mid([u_0])$), then the enclosure has the width

$$w([u_1]) = \left| \frac{\partial \Psi}{\partial u}([u_0]; h) \right| w([u_0]) + w([r]).$$

(The width of a vector is taken componentwise. It is a vector again. The absolute value of a matrix is taken elementwise: $|A| := (|a_{ij}|)$.) In some cases, the mean-value evaluation is width-decreasing. However, we have $w([u_1]) \geq w([r])$ in every case. Clearly, this holds for every method using inclusion (2).

3 An implicit method

This section deals with a new enclosure strategy. It is also based on Taylor expansion, but it uses a different enclosure principle. Let there be given the coarse enclosure $[U]$ from above. Then we have

$$u_0 \in \Psi(u(t_1); -h) + [r^-] \tag{4}$$

with

$$[r^-] = \frac{(-h)^{p+1}}{(p+1)!} f^{(p+1)}([U]) = \begin{cases} [r]\,, & p \ odd \\ -[r]\,, & p \ even \end{cases} .$$

The sought value $u(t_1)$ appears implicitly in (4). Classical implicit single step methods often work better than explicit ones do, particularly for stiff systems. This is our motivation to derive an implicit enclosure method which uses formula (4) instead of (2) for verification.

There is a real vector $r^- \in [r^-]$ satisfying

$$u_0 = \Psi(u(t_1); -h) + r^- .$$

Hence, $u(t_1)$ is a zero of the function $g : [U] \to I\!R^n$ with

$$g(v) = \Psi(v; -h) - u_0 + r^- .$$

Since we do not know the vectors u_0 and r^- exactly, we have to restrict our considerations on the interval function

$$[g](v) := \Psi(v; -h) - [u_0] + [r^-].$$

The solution $u(t_1)$ fulfils the relation

$$u(t_1) \in [v] := \bigsqcup \{v \in [U] \,|\, 0 \in [g](v)\},$$

where $\bigsqcup A$ denotes the interval hull of the set $A \subseteq I\!R^n$.

In general, we cannot compute the interval vector $[v]$ exactly. However, we can obtain a (hopefully) tight enclosure of $[v]$ by applying a Newton-like method. The following theorem can easily be proved.

Theorem 1. *Let the interval matrix $[\partial\Psi^-] := \dfrac{\partial \Psi}{\partial u}([U]; -h)$ be regular (i.e. every real matrix $A \in [\partial\Psi^-]$ is regular) and let $[\partial\Psi^-_{inv}]$ be an interval matrix with $A^{-1} \in [\partial\Psi^-_{inv}]$ for all $A \in [\partial\Psi^-]$. Let the sequence $[J_0], [J_1], [J_2], \ldots$ be given by the recursion formula*

$$[J_0] := [U],$$

$$[J_{k+1}] := (\hat{J}_k - [\partial\Psi^-_{inv}][g](\hat{J}_k)) \cap [J_k] \tag{5}$$

$$\textit{for some } \hat{J}_k \in [J_k] \textit{ and for } k = 0, 1, 2, \ldots .$$

Then we have
a) $[J_{k+1}] \subseteq [J_k]$ and $[v] \subseteq [J_k]$ for all $k = 0, 1, 2, \ldots$,
b) $[J_{k+1}] \neq [J_k]$ if $0 \notin [\partial\Psi^-_{inv}][g](\hat{J}_k)$.

The implicit method is given by Algorithm (5) (with $\hat{J}_k = mid([J_k])$ for instance) supplied with a stopping criterion, eg: "Repeat (5) until $[J_{k+1}] = [J_k]$ or $0 \in [g](\hat{J}_k)$." (On a computer, we always reach $[J_{k+1}] = [J_k]$ after a finite number of steps.) It can easily be worked into a computer code for an explicit Taylor method since both algorithms can use the same tools for the evaluation of the expressions Ψ and $\partial\Psi/\partial u$.

Of course, Algorithm (5) does not always yield satisfactory results. It is of no use if $[J_1]$ and $[J_0]$ are identical. Furthermore, the assumptions in Theorem 1 are very restrictive. $[U]$ is a coarse enclosure of $u(t)$ on $[t_0, t_1]$. The "inversion" of $[\partial\Psi^-]$ often fails due to the wide bounds of $[U]$. However, it is sufficient to use an enclosure of u at t_1 only. Theorem 1 keeps valid if we define $[\partial\Psi^-] := \frac{\partial\Psi}{\partial u}([u]; -h)$ and $[J_0] := [u]$, where $[u]$ is an enclosure of $u(t_1)$ calculated by an explicit Taylor method, for instance. Hence, the implicit method can be used as a corrector. If the first Newton step does not improve the enclosure of the predictor significantly, then one can use the coefficients of the polynomials $\Psi(\hat{u}; -h)$ and $\frac{\partial\Psi}{\partial u}([u]; -h)$ for the next (explicit) integration step. In this case, the additional costs of the corrector step are small since the calculation of these coefficients causes the major costs in both (explicit and implicit) methods.

A variety of methods could be derived from Algorithm (5), which is just a prototype. In the present formulation, Algorithm (5) can already be used to compute enclosures on a grid $\{t_1, t_2, \ldots, t_m\}$. However, it does not yet take account of the wrapping effect.

4 Linear systems

In this section, we apply explicit and implicit methods to linear ODE systems with constant coefficients and compare the results. We consider the problem

$$u' = Au, \quad u(0) = u_0 \in [u_0]$$

with $A \in IR^{n\times n}$. Let I denote the identity matrix and let us again assume that we know a coarse enclosure $[U]$ of the solution $u(t)$ on the interval $[0, h]$. Then we have

$$\Psi(u; h) = u + \sum_{j=1}^{p} \frac{1}{j!}(hA)^j u,$$

$$\frac{\partial\Psi}{\partial u}(u; h) = I + \sum_{j=1}^{p} \frac{1}{j!}(hA)^j =: B,$$

$$[r] = \frac{1}{(p+1)!}(hA)^{p+1}[U].$$

The mean-value method (3) yields the enclosure

$$u(h) \in [u] := B\hat{u}_0 + B([u_0] - \hat{u}_0) + [r] = B[u_0] + [r]$$

since B is a real matrix without any interval entries. The width of $[u]$ is

$$w([u]) = |B| w([u_0]) + w([r]). \tag{6}$$

In the implicit method, we can compute the interval hull $[v]$ of $\{v \in [U] \mid 0 \in [g](v)\}$ (see Section 3) by performing only one Newton step since the problem is linear. We get

$$[\partial\Psi^-] = \frac{\partial\Psi}{\partial u}([U]; -h) = I + \sum_{j=1}^{p} \frac{1}{j!}(-hA)^j =: C,$$

$$[\partial\Psi^-_{inv}] = C^{-1},$$

$$[r^-] = \frac{1}{(p+1)!}(-hA)^{p+1}[U] = \begin{cases} [r]\,, & p \ odd \\ -[r]\,, & p \ even \end{cases},$$

and finally

$$\begin{aligned} u(h) \in [v] &= (\hat{u} - C^{-1}[g](\hat{u})) \cap [U] \quad \text{(for some } \hat{u} \in [U]) \\ &= (\hat{u} - C^{-1}(C\hat{u} - [u_0] + [r^-])) \cap [U] \\ &= C^{-1}([u_0] - [r^-]) \cap [U]. \end{aligned}$$

Since $[r^-]$ has the same width as $[r]$, the width of the "implicit enclosure" is

$$w([v]) = |C^{-1}|(w([u_0]) + w([r])) \tag{7}$$

(or even smaller if $C^{-1}([u_0] - [r^-]) \not\subseteq [U]$). In Section 2, we saw that explicit Taylor methods always yield enclosures $[u]$ with $w([u]) \geq w([r])$. This does not hold for implicit methods. They sometimes reduce the width of the error term.

Below, some examples are shown. For given matrices A, initial values $[u_0]$, coarse enclosures $[U]$, step sizes h, and orders p, we evaluate the formulae (6) and (7). w_{ex} and w_{im} denote the maxima of the components of $w([u])$ and $w([v])$, respectively.

Example 1. [Grigorieff 72]

$$A = \begin{pmatrix} -50.5 & 49.5 \\ 49.5 & -50.5 \end{pmatrix}, \quad u_0 = \begin{pmatrix} 3 \\ 1 \end{pmatrix}, \quad [U] = \begin{pmatrix} [0,3] \\ [0,2] \end{pmatrix}.$$

h	0.1	0.1	0.3	0.3
p	30	50	80	100
w_{ex}	3.0E-3	1.6E-15	1.9E-1	4.1E-11
w_{im}	2.8E-3	1.5E-15	1.4E-1	3.0E-11

$$\text{Solution:} \quad u(t) = \begin{pmatrix} 2e^{-t} + e^{-100t} \\ 2e^{-t} - e^{-100t} \end{pmatrix}.$$

Example 2.

$$A = \begin{pmatrix} -50.5 & 49.5 \\ -49.5 & -50.5 \end{pmatrix}, \quad u_0 = \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad [U] = \begin{pmatrix} [-2,2] \\ [-2,2] \end{pmatrix}.$$

h	0.1	0.3	0.5	0.5
p	30	50	90	100
w_{ex}	1.4E-7	1.4E+2	2.7E+1	1.3E-3
w_{im}	1.1E-9	5.4E-5	3.8E-10	1.8E-14

$$\text{Solution:} \quad u(t) = e^{-50.5t} \begin{pmatrix} \sin 49.5t + \cos 49.5t \\ -\sin 49.5t + \cos 49.5t \end{pmatrix}.$$

Example 3.

$$A = \begin{pmatrix} -50.5 & 49.5 \\ -49.5 & -50.5 \end{pmatrix}, \quad [u_0] = \begin{pmatrix} [0,1] \\ [0,1] \end{pmatrix}, \quad [U] = \begin{pmatrix} [-2,2] \\ [-2,2] \end{pmatrix}.$$

h	0.1	0.3	0.5	0.5
p	30	50	90	100
w_{ex}	7.7E-3	1.7E+2	3.3E+1	1.1E-2
w_{im}	7.7E-3	5.4E-5	3.9E-10	1.4E-11

Example 4.

$$A = \begin{pmatrix} -1 & 0 \\ 0 & -100 \end{pmatrix}, \quad u_0 = \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad [U] = \begin{pmatrix} [0,2] \\ [0,2] \end{pmatrix}.$$

h	0.1	0.1	0.3	0.5
p	30	50	80	120
w_{ex}	2.4E-3	1.3E-15	1.5E-1	9.3E+4
w_{im}	1.1E-7	5.9E-20	1.4E-14	1.8E-17

$$\text{Solution:} \quad u(t) = \begin{pmatrix} e^{-t} \\ e^{-100t} \end{pmatrix}.$$

Example 1 is a stiff problem. The matrix A has the eigenvalues $\lambda_1 = -1$ and $\lambda_2 = -100$. Nevertheless, the implicit and the explicit method both yield nearly the same results. This does not hold for Example 2. Here, the implicit method works much better than the explicit one though the new problem is not stiff. The real part of both eigenvalues is $\mathrm{Re}(\lambda) = -50.5$. Example 3 shows the results for nearly the same problem, where only the initial value u_0 from Example 2 is replaced by an interval vector. Example 4 is again stiff. The matrices of Example 4 and Example 1 are similar. Particularly, they have the same eigenvalues and the same degree of stiffness. In contrast to Example 1, however, Example 4 shows a significant difference between the widths w_{im} and w_{ex}.

Obviously, the difference between the results of implicit and explicit methods does not depend on the degree of stiffness alone. Let us regard the formulae (6) and (7) for an explanation. For fixed h and p, the eigenvalues of B and C^{-1} are determined by the eigenvalues of A. However, this does not hold for the eigenvalues of the matrices $|B|$ and $|C^{-1}|$. Hence, we cannot expect similar matrices to yield similar results.

5 A nonlinear example

Finally, we consider a simple nonlinear example with some remarkable properties. The solution of

$$u' = -u^2, \quad u(1) = 1$$

is $u(t) = 1/t$. Using the coarse enclosure $[U] = [0,1]$, we get

$$\Psi(u_0;h) = \Psi(1;h) = \sum_{j=0}^{p}(-h)^j \quad \text{and} \quad [r] = (-h)^{p+1}[0,1].$$

None of the explicit methods mentioned in Section 2 is able to improve the coarse enclosure if they use a step size $h \geq 1$. On the other hand, it can be shown that the implicit method can yield tighter bounds for arbitrarily high step sizes.

If we replace the initial condition by $u(1) \in [0,1]$, then the set of all solutions is the interval function $[u](t) = [0, 1/t]$. The coarse enclosure $[U] = [0,1]$ is still valid for all $t \geq 1$. We applied the implicit method, described in Section 3, to this problem using $\hat{J}_k = mid([J_k])$ and the stopping criterion: "Repeat (5) until $[J_{k+1}] = [J_k]$". Some results are shown in the following table, in which $[v]$ denotes the enclosure calculated on a computer. $[u](t)$ is the actual solution set.

h	7	7	9	9	99	999
p	5	100	5	100	8	9
$[v]$	[0,0.249]	[0,0.1250014]	[0,0.125]	[0,0.125]	[0,0.0157]	[0,0.00196]
$[u](t)$	[0,0.125]	[0,0.125]	[0,0.1]	[0,0.1]	[0,0.01]	[0,0.001]

The Newton iteration causes some strange effects which heavily depend on the step size h. For particular sizes (eg. $h = 7$), we get an improvement of the results when the order p increases. In other cases, the minimal width of $[v]$ is reached for very small orders. Though these enclosures are not tight, they show the qualitative behaviour of the solution set. In contrast, every explicit method yields useless results for $h \geq 1$. For any order p, we only get supersets of the interval $[0,1]$. This is the coarse enclosure $[U]$ which is already known.

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