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Interval methods for initial value problems in ODEs

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1. Introduction

The treatment of differential equations is one of the main topics in numerical analysis. The current chapter deals with ordinary differential equations with initial conditions. Many methods are known to solve initial value problems approximately. If certain smoothness conditions are fulfilled, one can obtain sufficiently good approximations in theory by using some single- or multi-step method with sufficiently small stepsizes. However, in practice one seldom knows the suitable sizes. Even by applying a stepsize control, the global accuracy is not really controlled. After a few steps, the error may grow beyond all bounds. This is impressively demonstrated in [2] and [3] where Adams *et al.* show several examples in which the computed results do not even reflect the qualitative stability properties of the true solutions.

In contrast with approximate methods, enclosure methods yield verified results. That is, they assure the existence of a unique solution, and they yield either validated bounds of the true solution or validated bounds of the error of an approximate solution. At worst, the validation of the existence may fail or the bounds may be unacceptably wide. However, a correctly implemented enclosure method never yields a false result.

One uses interval arithmetic to implement enclosure methods. Interval methods are well suitable for implementation on a digital computer because all round-off errors, which are unavoidable in digital computations, can automatically be taken into account and enclosed by using machine interval arithmetic. The programming languages PASCAL-XSC, FORTRAN-XSC, and C-XSC (for instance) provide interval operations and interval evaluations of standard functions (sin, cos, exp, ln, ...) (see eg [39, 40]).

In 1965, Moore [52–54] described an enclosure method for ordinary differential equations using interval arithmetic for the first time. However, other approaches to generate error bounds of approximate solutions had already been developed before. One can estimate the error in a Picard-Lindelöf iteration using the fixed point theorem of Banach or Weissinger (see eg [30]). In the eighties, Moore [56], Nickel [62], Stetter [84], Bauch *et al.* [13], and Corliss [20] gave surveys on interval methods available by then. In Corliss *et al.* [21], one can find a very extensive bibliography.

Below we give a survey of the most commonly used approaches. Section 2 contains the description of the problem and some preliminary remarks. In Section 3 we list some basic inclusion theorems for the verification of solutions. We then discuss several enclosure methods which are based on the following three principles:

(A) *Improve the bounds of a provisional inclusion iteratively* (iterative methods),

(B) *Bound the error of a "good" continuous approximate solution* (continuous error methods),

(C) *Bound the truncation error of a single-step method* (discrete error methods).

Section 4 deals with *iterative methods.* Moore introduces an interval Picard-Lindelöf iteration in [53]. Bauch and others [11, 13] modify the method and suggest a Newton iteration. In Section 5 we handle the principle of *continuous error methods.* One computes a continuous approximation and estimates the error using some results of the theory of differential inequalities. Marcowitz [51] presents a very sophisticated method based on some ideas of Walter [90] and Schröder [78, 79].

Iterative methods (Section 4) as well as *continuous error methods* (Section 5) require "continuous calculations". They deal with real functions which have to be integrated or differentiated formally. In contrast, *discrete error methods* (Section 6) use function evaluations at some discrete points and intervals and yield narrow continuous inclusions nonetheless. This is an important point concerning practical implementation. The discrete methods we discuss in Section 6 and Section 8 are based on the pioneering work of Moore [52–54]. They use Taylor series expansions and estimations of the local truncation errors.

Every interval method has to face the so-called *wrapping effect* introduced in Section 7. It often causes large overestimations of the error bounds. One can avoid the wrapping effect in some special cases. However, it is a severe obstacle in enclosure methods in general. We study the wrapping effect in interval Taylor series methods in Section 8. Moore [53, 54], Krückeberg [41], Eijgenraam [23], and Lohner [46, 47] present modifications of the Taylor method which can reduce the wrapping effect. The method of Lohner is the most famous one. It is implemented in the computer program AWA (Anfangswertaufgabe) which is used worldwide. We derive a similar method and discuss the quality of the error bounds.

Section 9 concludes the paper with some final remarks on applications, generalizations, and future research.

2. Preliminaries

We consider the *initial value problem*

$$u' = f(t,u), \quad u(t_0) = u_0 \tag{1}$$

with $t_0 < T \in \mathbb{R}$, $u_0 \in int(D)$, $D \in V_n(I(\mathbb{R}))$, and $f \in C([t_0,T] \times D, V_n(\mathbb{R}))$, i.e. $f : [t_0,T] \times D \to V_n(\mathbb{R})$ is a continuous function. Furthermore, we suppose that the partial derivatives $\dfrac{\partial f}{\partial u_{(i)}}$ of f with respect to the components $u_{(i)}$ of u exist and are continuous in $[t_0,T] \times D$. Then there is a unique solution $u^*(t)$ of (1). It exists at least on an interval $[t_0,\hat{t}]$ with $\hat{t} = T$ or $u^*(\hat{t}) \in \partial D$ (and $t_0 < \hat{t} < T$), respectively (see eg [91]). An explicit differential equation of higher order can always be transformed into a system of first order equations.

It is well known that $u^*(t)$ is the unique solution of the *integral equation*

$$u(t) = u_0 + \int_{t_0}^{t} f(\tau, u(\tau))d\tau \tag{2}$$

as well (see eg [30, 91]).

Sometimes we do not know the exact initial value u_0 but only an interval inclusion $[u_0] \subseteq D$ of it. Let $[v] \subseteq D$ be an interval vector and $s, \hat{s} \in [t_0, T]$. Then $\{u(\hat{s}; s, [v])\}$ denotes the set of the solutions of all initial value problems

$$u' = f(t, u), \quad u(s) = v$$

with $v \in [v]$, evaluated at $\hat{s}$, provided that they exist at $\hat{s}$. Then we have $u^*(t) \in \{u(t; t_0, [u_0])\}$ for $u_0 \in [u_0]$.

We require the function f to have a *finite representation*. That means, the given expression of f consists of a combination of a finite number of constants, variables, elementary operations, and standard functions. Then one can evaluate f approximately by performing a finite sequence of operations on a computer. One can enclose the value of f by using interval arithmetic. We always require the interval evaluation of a function with a finite representation to be inclusion monotonic ($[x] \subseteq [y] \Rightarrow f([x]) \subseteq f([y])$). For a rigorous analysis of interval evaluation, see Neumaier [57].

If the expression of f contains some "constant intervals" $[c_1], [c_2], \ldots, [c_k]$, Bauch, Kimmel [14], and Lohner [46] replace them by k additional variables $u_{(n+1)}, u_{(n+2)}, \ldots, u_{(n+k)}$ and hence get k additional differential equations $u'_{(n+i)} = 0$ with the initial conditions $u_{(n+i)}(t_0) = c_i$, $c_i \in [c_i]$, $i = 1, 2, \ldots, k$. Thus, one again obtains an initial value problem (1) with a real vector-valued f and an initial interval vector $[u_0]$.

A sensible numerical treatment of our problem mostly requires the splitting of the interval $[t_0, T]$ into many subintervals $[t_0, t_1], [t_1, t_2], \ldots, [t_{m-1}, t_m]$. Classical (non-interval) methods compute approximations on the grid intervals or at least at the grid points $t_1, t_2, \ldots, t_m$, successively.

Let $\tilde{u} : [t_0, \tilde{t}] \to D$ ($\tilde{t} \in (t_0, T]$) be a continuously differentiable approximate solution of (1), $e(t) := u^*(t) - \tilde{u}(t)$ be the error, and $d(t) := f(t, \tilde{u}(t)) - \tilde{u}'(t)$ be the defect. Then $e(t)$ is the unique solution of the error problem

$$e' = f(t, \tilde{u}(t) + e) - f(t, \tilde{u}(t)) + d(t), \quad e(t_0) = u_0 - \tilde{u}(t_0). \tag{3}$$

If we only have a pointwise approximation $\tilde{u}_0, \tilde{u}_1, \ldots, \tilde{u}_m$ at the grid points $t_0, t_1, \ldots, t_m$, then we define $e_j := u^*(t_j) - \tilde{u}_j$, provided that $u^*(t_j)$ exists ($j = 0, 1, \ldots, m$).

We will not go into classical approximate methods. We want to compute inclusions of $u^*(t)$ instead of approximations. Using an inclusion $[u_{j-1}]$ of $u^*(t_{j-1})$, we seek a *continuous inclusion* $[u](t)$ ($= \tilde{u}(t) + [e](t)$) with continuous bounds $\underline{u}(t)$ and $\overline{u}(t)$ ($\underline{e}(t)$ and $\overline{e}(t)$) and with $u^*(t) \in [u](t) \subseteq D$ for $t \in [t_{j-1}, t_j]$ or at least a *point inclusion* $[u_j]$ ($= \tilde{u}(t_j) + [e_j]$) $\subseteq D$ with $u^*(t_j) \in [u_j]$. We start at $[u_0]$, and we step from one grid point to the other until the enclosure fails, D is left, or t_m is reached. In the following four sections we only consider a single step, i.e. the enclosure of the solution on the first interval $[t_0, t_1]$.

3. Basic error estimations and a priori inclusions

The computation of guaranteed solution bounds requires the application of some theoretical results. That means, every verification process is based on some existence and inclusion theorems. Some of the following results are not useful for the computation of tight bounds. However, one can use them in order to verify a solution between some (wide) *a priori* bounds which may be improved by other methods.

Let us first consider the integral equation (2). It is a fixed point problem which can be solved by successive iteration. It is known that the *Picard-Lindelöf iteration*

$$u_{k+1}(t) := u_0 + \int_{t_0}^{t} f(\tau, u_k(\tau))d\tau, \quad k = 1, 2, \ldots \tag{4}$$

yields a sequence of functions which converge to the unique solution u^* on $[t_0, t_1]$ provided that $u_1(t)$ is continuous and the whole sequence lies in D for $t \in [t_0, t_1]$ (see eg [30, 91]). The error estimation in the Theorem of Picard-Lindelöf (see eg [30]) yields

Theorem 3.1 *Let $[u] \subseteq D$ be an interval vector and let $u_1(t)$ be a continuous function with $u_1(t) \in \mathrm{int}([u])$ for $t \in [t_0, t_1]$. Assume that f satisfies a Lipschitz condition*

$$\|f(t,u) - f(t,v)\|_\infty \leq L\|u - v\|_\infty \quad \textit{for } t \in [t_0, t_1],\ u, v \in [u]$$

with a positive constant L with $\alpha := (t_1 - t_0)L < 1$. ($\|.\|_\infty$ denotes the maximum norm.) If the inclusion

$$[\hat{u}](t) := u_2(t) + \frac{\alpha}{1-\alpha} \max_{\tau \in [t_0,t_1]} \|u_2(\tau) - u_1(\tau)\|_\infty [i] \subseteq [u]$$

is valid for $t \in [t_0, t_1]$ with $[i] := ([-1,1], [-1,1], \ldots, [-1,1])^{\mathrm{T}} \in V_n(I(\mathbf{R}))$ and $u_2(t)$ defined by (4), then the solution u^* of (1) exists on $[t_0, t_1]$ and

$$u^*(t) \in [\hat{u}](t) \quad \textit{for} \quad t \in [t_0, t_1].$$

Remark: In general, $[\hat{u}]$ is not the tightest inclusion one can obtain by using L and u_1. However, we do not want to list all possible estimations. We only want to show some representative but simple examples of various principles.

If $(t_1 - t_0)$ is small enough, one can satisfy the conditions of Theorem 3.1 and one already gets an inclusion of u^* by performing a single step of the Picard-Lindelöf iteration. Bachmann follows this idea in [8]. However, he uses more sophisticated estimations and some additional methods to improve the inclusions. If one knows an estimation of the norm of f instead of a Lipschitz constant L, one can verify an inclusion of u^* using

Theorem 3.2 *Let $[u_0]$ be an inclusion of u_0 with $[u_0] \subseteq \mathrm{int}([u]) \subseteq D$. Assume that f satisfies*

$$\|f(t,u)\|_\infty \leq K \quad \textit{for } t \in [t_0, t_1],\ u \in [u]$$

with a positive constant K. If the inclusion

$$[\hat{u}](t) := [u_0] + (t - t_0)K[i] \subseteq [u]$$

is valid for $t \in [t_0, t_1]$, then u^* exists on this interval, and

$$u^*(t) \in [\hat{u}](t) \quad \textit{for} \quad t \in [t_0, t_1].$$

One can satisfy the required inclusion by reducing the stepsize $h := t_1 - t_0$.

We do not need L or K if we use *interval integration*. Let us define the integral of an interval (vector) valued function $[g](t)$ with continuous bounds $\underline{g}(t)$ and $\overline{g}(t)$ by

$$\int_a^t [g](\tau)d\tau := \left[\int_a^t \underline{g}(\tau)d\tau, \int_a^t \overline{g}(\tau)d\tau\right]. \tag{5}$$

Then we have

$$\int_a^t g(\tau)d\tau \in \int_a^t [g](\tau)d\tau$$

for each continuous function $g(t) \in [g](t)$. Moreover, the interval operation (5) is inclusion monotonic (see also Moore [55]).

Kaucher and Miranker [36] present the concept of the *ultra-arithmetic*. They provide machine operations for the formal integration of every linear combination of a finite number of "basis functions" (eg polynomials). On a computer the combinations are represented by their coefficients. We get interval functions if the coefficients are intervals. However, one has to be very careful with the formal integration of functions with interval coefficients or interval parameters. For example, we have

$$\int_{-1}^{1} [c]t \; dt = \frac{1}{2}([c] - [c]) \neq 0 = [c] \int_{-1}^{1} t \; dt$$

if $[c]$ is a non-degenerate interval.

Theorem 3.3 *Let $[u_0]$ be an inclusion of u_0, let $[u](t)$ be an interval vector valued function with continuous bounds, and let $[u](t) \subseteq D$ for $t \in [t_0, t_1]$. If the inclusion*

$$[\hat{u}](t) := [u_0] + \int_{t_0}^{t} f(\tau, [u](\tau))d\tau \subseteq [u](t) \tag{6}$$

holds for $t \in [t_0, t_1]$, then u^* exists on this interval and

$$u^*(t) \in [\hat{u}](t) \quad \textit{for} \quad t \in [t_0, t_1].$$

One can prove Theorems 3.2 and 3.3 easily by showing that the whole sequence $\{u_k(t)\}_{k=2}^{\infty}$ defined by (4) is included in $[\hat{u}](t)$ if $u_1(t) \in [u]$ (in 3.2) or $u_1(t) \in [u](t)$ (in 3.3), respectively.

Later we will consider some methods which do not require more than a *constant inclusion* (i.e. an inclusion with constant bounds on the whole interval $[t_0, t_1]$) in order to compute very tight error bounds finally. One can check the validity of a constant inclusion without using any integration by

Corollary 3.4 (see also Lohner [46, 47]) *If the inclusion*

$$[\hat{u}] := [u_0] + [0,h]f([t_0,t_1],[u]) \subseteq [u] \tag{7}$$

holds with $u_0 \in [u_0] \subseteq [u] \subseteq D$ *and* $h := t_1 - t_0$, *then* u^* *exists on* $[t_0,t_1]$ *and*

$u^*(t) \in [\hat{u}]$ *for* $t \in [t_0,t_1]$.

The following algorithm gives a constructive method to generate a constant inclusion. Lohner [47] has implemented it in his program AWA mentioned in section 1.

Algorithm 1

(i) *Set* $[\tilde{u}] := [u_0]$,

(ii) *produce an* inflation $[u]$ *of* $[\tilde{u}]$, *i.e. an enlarged interval* $[u]$ *containing* $[\tilde{u}]$ *in its interior, and*

(iii) *compute* $[\tilde{u}] := [u_0] + [0,h]f([t_0,t_0+h],[u])$.

(iv) *If* $[\tilde{u}] \subseteq [u]$ *go to* (v).

Otherwise, you have two possibilities to continue :

a) decrease h *and go to* (i) *or*

b) go to (ii).

(v) $[\hat{u}] := [\tilde{u}]$.

Remark: On a digital computer, the finiteness of the machine numbers limits the reduction of h. The algorithm may fail. That means, it does not succeed in finding an inclusion of u^*. This difficulty appears in every method. It is not guaranteed that we obtain any result at all, but if we do, then the result is verified.

Instead of a constant inclusion, one can also obtain a *linear inclusion* by replacing $[0,h]$ by $(t-t_0)$ in (7):

$$[\hat{u}](t) := [u_0] + (t-t_0)f([t_0,t_1],[u]) \subseteq [u]. \tag{8}$$

Below, we give some alternatives of the inclusion condition (6) in Theorem 3.3. We can use the *mean-value evaluation*

$$f_M(\tau,[u](\tau)) = f(\tau,\tilde{u}(\tau)) + \frac{\partial f}{\partial u}(\tau,[u](\tau))([u](\tau)-\tilde{u}(\tau))$$

with $\tilde{u}(t) \in [u](t)$ for $t \in [t_0,t_1]$ instead of the direct interval evaluation $f(\tau,[u](\tau))$ of f. (Kaucher and Miranker use this idea in [36].) (6) turns into

$$[\hat{u}](t) := [u_0] + \int_{t_0}^{t} f(\tau,\tilde{u}(\tau))d\tau + \int_{t_0}^{t} \frac{\partial f}{\partial u}(\tau,[u](\tau))([u](\tau)-\tilde{u}(\tau))d\tau \subseteq [u](t). \tag{9}$$

The statement of 3.3 remains true. This can be shown by using the mean-value theorem (for every single component). In [11–13] Bauch uses inclusion conditions which even contain the second partial derivatives of f. However, interval integration always requires the determination of the bounds of the integrand.

If f is *monotone* in u (i.e. f is increasing in each component of u), we can replace (6) by

$$\begin{aligned} \underline{\hat{u}}(t) &:= \underline{u}_0 + \int_{t_0}^{t} f(\tau, \underline{u}(\tau))d\tau \geq \underline{u}(t), \\ \overline{\hat{u}}(t) &:= \overline{u}_0 + \int_{t_0}^{t} f(\tau, \overline{u}(\tau))d\tau \leq \overline{u}(t). \end{aligned} \tag{10}$$

($\leq, \geq$ have to be taken componentwise.) Again we get $u^*(t) \in [\hat{u}](t) = [\underline{\hat{u}}(t), \overline{\hat{u}}(t)]$ for $\underline{u}_0 \leq u_0 \leq \overline{u}_0$, $[\underline{u}(t), \overline{u}(t)] \subseteq D$.

However, the monotonicity of f is a very restrictive assumption. For more general functions, one can find two continuous functions $g_i : [t_0, t_1] \times D \times D \to V_n(\mathbf{R})$, $i = 1, 2$ with

$$g_1(t, u, u) \leq f(t, u) \leq g_2(t, u, u) \quad \text{for} \quad t \in [t_0, t_1], \quad u \in D,$$

where $g_i(t, u, v)$ is monotone in u and *antitone* in v (i.e. decreasing in each component of v). Then one has to replace (10) by

$$\begin{aligned} \underline{\hat{u}}(t) &:= \underline{u}_0 + \int_{t_0}^{t} g_1(\tau, \underline{u}(\tau), \overline{u}(\tau))d\tau \geq \underline{u}(t), \\ \overline{\hat{u}}(t) &:= \overline{u}_0 + \int_{t_0}^{t} g_2(\tau, \overline{u}(\tau), \underline{u}(\tau))d\tau \leq \overline{u}(t). \end{aligned} \tag{11}$$

If $g_1(t, u, v) = g_2(t, u, v)$ for $u, v \in D$, then f is called *monotone decomposable* (see eg Schröder [81]). If we want to validate the inequalities in (10) or (11) on a computer, we have to use directed rounding though no intervals appear.

We now consider the original initial value problem (1) instead of the integral equation (2). That means, we deal with the derivatives of approximate solutions or solution bounds instead of the integral of f. Unfortunately, interval valued functions cannot be differentiated since the range of the derivatives of all differentiable functions included in a non-degenerate interval function is not bounded. Nevertheless, one can give a sufficient condition for the derivatives of the bounds to satisfy (6).

Corollary 3.5 *If $u_0 \in [u](t_0)$, $[u](t) = [\underline{u}(t), \overline{u}(t)] \subseteq D$ with continuously differentiable bounds $\underline{u}(t), \overline{u}(t)$ and if the inequalities*

$$\underline{u}'(t) \leq f(t, v) \leq \overline{u}'(t) \quad \textit{for} \quad v \in [u](t) \tag{12}$$

hold for $t \in [t_0, t_1]$, then

$$u^*(t) \in [u](t) \quad \textit{for} \quad t \in [t_0, t_1].$$

This can be shown by integration.

If f is monotone, we can replace (12) by

$$\underline{u}'(t) \leq f(t, \underline{u}(t)), \quad f(t, \overline{u}(t)) \leq \overline{u}'(t). \tag{13}$$

However, Walter [90] shows that some weaker assumptions than the monotonicity are sufficient as well. f is called *quasimonotone* in u if every component $f_{(i)}(t, u)$ $(i = 1, 2, \ldots, n)$ is monotone in each component $u_{(k)}$ of u with $k \neq i$, i.e.

$$f_{(i)}(t, u) \leq f_{(i)}(t, v) \quad \text{for} \quad u \leq v, \quad u_{(i)} = v_{(i)}$$

and for $i = 1, 2, \ldots, n$.

Theorem 3.6 (Walter [90]) *Let $f(t, u)$ be quasimonotone in u for $(t, u) \in [t_0, t_1] \times D$, and let $[u](t) = [\underline{u}(t), \overline{u}(t)] \subseteq D$ $(t \in [t_0, t_1])$ be an interval vector valued function with continuously differentiable bounds $\underline{u}, \overline{u}$ which satisfies $u_0 \in [u](t_0) \subseteq D$ and*

$$\underline{u}'(t) \leq f(t, \underline{u}(t)), \quad f(t, \overline{u}(t)) \leq \overline{u}'(t) \quad \textit{for} \quad t \in [t_0, t_1].$$

Then $u^*(t)$ exists on this interval and

$$u^*(t) \in [u](t) \quad \textit{for} \quad t \in [t_0, t_1].$$

Every scalar function $f(t, u)$ $(u \in \mathbf{R})$ is quasimonotone in u. For arbitrary functions f (continuously differentiable as usual but not necessarily quasimonotone), we have

Theorem 3.7 (Schröder [80]) *Let $[u](t) = [\underline{u}(t), \overline{u}(t)] \subseteq D$ $(t \in [t_0, t_1])$ be an interval vector valued function with continuously differentiable bounds $\underline{u}$, $\overline{u}$ which satisfies $u_0 \in [u](t_0) \subseteq D$. If the inequalities*

$$\underline{u}'_{(k)}(t) \leq f_{(k)}(t, v) \quad \textit{for} \quad v \in [u](t), \quad v_{(k)} = \underline{u}_{(k)}(t)$$

and

$$\overline{u}'_{(k)}(t) \geq f_{(k)}(t, v) \quad \textit{for} \quad v \in [u](t), \quad v_{(k)} = \overline{u}_{(k)}(t)$$

hold for $k = 1, 2, \ldots, n$ and $t \in [t_0, t_1]$, then $u^*(t)$ exists on this interval and

$$u^*(t) \in [u](t) \quad \textit{for} \quad t \in [t_0, t_1].$$

One can sometimes estimate u^* by solving a "neighbouring" initial value problem. Let f be linear in u:

$$f(t, u) = A(t)u + g(t)$$

with continuous functions $g : [t_0, t_1] \to V_n(\mathbf{R})$ and $A : [t_0, t_1] \to M_{nn}(\mathbf{R})$. If two other continuous functions $h : [t_0, t_1] \to V_n(\mathbf{R})$ and $K : [t_0, t_1] \in M_{nn}(\mathbf{R})$ satisfy $|g(t)| \leq h(t)$, $A_{ii}(t) \leq K_{ii}(t)$ and $|A_{ik}(t)| \leq K_{ik}(t)$ for $i, k = 1, 2, \ldots, n$ and $i \neq k$, $t \in [t_0, t_1]$, then

$$F(t, u) := K(t)u + h(t)$$

is quasimonotone, and we get

Corollary 3.8 *On the above conditions for h and K, every continuously differentiable function $v(t)$ with*

$$F(t,v) \le v', \quad |u_0| \le v(t_0)$$

satisfies

$$|u^*(t)| \le v(t) \quad \textit{for} \quad t \in [t_0, t_1].$$

(The absolute value of a vector or a matrix is taken componentwise and elementwise, respectively.) Uhlmann uses this corollary in [87], where he bounds the solution of a linearized form of the error problem (3).

The application of the theoretical results of this section requires the verification of some inclusions $[u](t) \subseteq [v](t)$ or inequalities $u(t) \le v(t)$ for all(!) $t \in [t_0, t_1]$. This is difficult in general. Corollary 3.4, however, is an important exception since we have no explicit dependence on t in its conditions. For further inclusion theorems see eg [44, 81, 90].

4. Improving an inclusion iteratively

Let us assume that we already have a continuous inclusion $[u](t)$ of the solution $u^*(t)$ on $[t_0, t_1]$. It may be a rough inclusion (eg a constant or a linear inclusion $[\hat{u}](t)$ satisfying (7) and (8), respectively) as well as a tight inclusion computed by some (arbitrary) enclosure method. In this section, we discuss iterative methods to improve $[u_1](t) := [u](t)$ step by step. They generate a finite sequence $\{[u_j](t)\}_{j=1}^{p}$ of interval vector valued functions with $u^*(t) \in [u_j](t)$ and

$$w([u_{j+1}](t)) \le w([u_j](t)) \quad \text{for} \quad t \in [t_0, t_1], \quad j = 1, 2, \ldots, p-1. \tag{14}$$

(The width $w([u])$ of an interval vector $[u] = [\underline{u}, \overline{u}]$ is the real vector $\overline{u} - \underline{u}$.)

Moore [53] describes an interval version of the *Picard-Lindelöf iteration*:

$$[u_{j+1}](t) := [u_0] + \int_{t_0}^{t} f(\tau, [u_j](\tau))\, d\tau, \quad j = 1, 2, \ldots, p-1. \tag{15}$$

For $j = 1, 2, \ldots, p$, we have $u^*(t) \in [u_j(t)]$. If the inclusion $[u_2](t) \subseteq [u_1](t)$ holds, then we even have $[u_{j+1}](t) \subseteq [u_j](t)$ for $j = 1, 2, \ldots, p-1$. (According to Theorem 3.3, $[u_2](t) \subseteq [u_1](t)$ implies $u^*(t) \in [u_1](t)$. If we can verify the first inclusion, we do not have to presuppose the second one.)

Assume that K is a positive constant with

$$w(f(t, [u])) \le K w([u]) \quad \text{for } t \in [t_0, t_1], \ [u] \subseteq [u_1](t),$$

and that $[u_0]$ is the point vector u_0. Let $w([u_j])$ denote the width

$$w([u_j]) := \max_{\tau \in [t_0, t_1]} w([u_j](\tau)).$$

Then we have

$$\begin{aligned} w([u_{j+1}]) &\le \int_{t_0}^{t_1} K\, w([u_j](\tau))\, d\tau \\ &\le (t_1 - t_0)\, K\, w([u_j]). \end{aligned}$$

For $(t_1 - t_0)K < 1$, the sequence $\{w([u_j])\}_{j=1}^{\infty}$ converges to zero at least linearly. That is, the bounds of $[u_j](t)$ converge to the solution $u^*(t)$ uniformly and at least linearly.

Of course, we have no convergence if $w([u_0]) \neq 0$ or if we use machine interval arithmetic. One has to modify the iteration in order to guarantee property (14) at least:

$$[u_{j+1}](t) := \left([u_0] + \int_{t_0}^{t} f(\tau, [u_j](\tau))\, d\tau \right) \cap [u_j](t).$$

One can replace the direct evaluation by the mean-value evaluation as in (9) and thus gets the iteration formula

$$[u_{j+1}](t) := \left([u_0] + \int_{t_0}^{t} \left(f(\tau, \tilde{u}_j(\tau)) + \frac{\partial f}{\partial u}(\tau, [u_j](\tau))([u_j](\tau) - \tilde{u}_j(\tau)) \right) d\tau \right) \cap [u_j](t)$$

with $\tilde{u}_j(t) \in [u_j](t)$. Bauch [13] even uses a *second order evaluation* of f (provided that the second partial derivatives of f with respect to u exist and are continuous):

$$\begin{aligned}[u_{j+1}](t) := \Bigg([u_0] \;+\; \int_{t_0}^{t} \Bigg(& f(\tau, \tilde{u}_j(\tau)) + \frac{\partial f}{\partial u}(\tau, \tilde{u}_j(\tau))([u_j](\tau) - \tilde{u}_j(\tau)) + \\ & q(\tau, [u_1](\tau), [u_j](\tau) - \tilde{u}_j(\tau)) \Bigg)\, d\tau \Bigg) \cap [u_j](t) \end{aligned} \tag{16}$$

with $\tilde{u}_j(t) \in [u_j](t)$. If $g(t)$ is a function with n components, then $q(t, u, g(t))$ denotes the vector function with the components

$$q_{(k)}(t, u, g(t)) = \frac{1}{2} g^T(t) \frac{\partial^2 f_{(k)}}{\partial u^2}(t, u) g(t), \quad k = 1, 2, \ldots, n. \tag{17}$$

The different evaluations of f yield different widths of the inclusions, generally. The optimal evaluation depends on f (or rather on the given expression of f) and on the inclusion $[u_j](t)$.

Each of the above methods require interval integration. One has to integrate continuous bounds of $f(t, u(t))$ for $u(t) \in [u_j](t)$. We can avoid interval functions if we know a *monotone decomposition* of f. Let us assume that $\tilde{f}(t, u, v) \in C([t_0, t_1] \times D \times D, V_n(\mathbf{R}))$ is monotone in u and antitone in v and fulfils $\tilde{f}(t, u, u) = f(t, u)$. Then one can replace (15) by

$$\begin{aligned} \underline{u}_{j+1}(t) &:= \underline{u}_0 + \int_{t_0}^{t} \tilde{f}(\tau, \underline{u}_j(\tau), \overline{u}_j(\tau)) d\tau, \\ \overline{u}_{j+1}(t) &:= \overline{u}_0 + \int_{t_0}^{t} \tilde{f}(\tau, \overline{u}^k(\tau), \underline{u}_j(\tau)) d\tau. \end{aligned}$$

An important special case is

$$\tilde{f}(t, u, v) = f^+(t, u) + f^-(t, v)$$

(i.e. f^+ is monotone and f^- is antitone) (see also Collatz [17] and Schröder [81]).

In [4] and [76], Adams and Scheu replace the original differential equation $u' = f(t,u)$ by

$$u' - \Omega u = f(t,u) - \Omega u =: g(t,u).$$

They choose the matrix $\Omega \in M_{nn}(\mathbf{R})$ in such a way that g is decreasing in u. They start with an inclusion $[u_1](t) = [\underline{u}_1(t), \overline{u}_1(t)]$ of the solution $u^*(t)$ and obtain a sequence of lower and upper bounds by the iteration

$$\begin{aligned}
\underline{u}_{j+1}(t) &= e^{\Omega t}\left(e^{-\Omega t_0}\underline{u}_0 + \int_{t_0}^{t} e^{-\Omega\tau} g(\tau, \overline{u}_j(\tau))\, d\tau\right), \\
\overline{u}_{j+1}(t) &= e^{\Omega t}\left(e^{-\Omega t_0}\overline{u}_0 + \int_{t_0}^{t} e^{-\Omega\tau} g(\tau, \underline{u}_j(\tau))\, d\tau\right).
\end{aligned}$$

One can replace $\underline{u}_j$ in the second equation by $\underline{u}_{j+1}$ in order to accelerate the method.

Ames and Ginsberg [6] consider some modifications of the Picard-Lindelöf integral operator which yield a sequence of alternately lower and upper bounds of the solutions of initial value problems with some particular monotonicity properties.

However, every *Picard iteration* converges only linearly, in general (provided that $[u_0] = u_0$ and round-off errors do not occur). Therefore, Bauch [11, 12] suggests *Newton's iteration*.

In Picard's iteration, one solves the "constant differential equations"

$$u'_{j+1} = f(t, u_j(t)).$$

In Newton's iteration, one solves the linear differential equations

$$u'_{j+1} = f(t, u_j(t)) + \frac{\partial f}{\partial u}(t, u_j(t))\,(u_{j+1} - u_j(t)).$$

Bauch presents an interval version of Newton's iteration for scalar differential equations in [11] and for systems in [12]. The latter one uses the implicit recursion formula

$$[v_j](t) := \left([u_0] + \int_{t_0}^{t} \left(f(\tau, \tilde{u}_j(\tau)) + \frac{\partial f}{\partial u}(\tau, [u_1](\tau))([u_j](\tau) - \tilde{u}_j(\tau)) \right) d\tau \right) \cap [u_j](t)$$

with $\tilde{u}_j(t) \in [u_j](t)$ (eg $\tilde{u}_j = m([u_j](t))$),

$$\begin{aligned}
[z_{j+1}](t) \;:=\; [u_0] + \int_{t_0}^{t} \Big(& f(\tau, \tilde{v}_j(\tau)) + \frac{\partial f}{\partial u}(\tau, \tilde{v}_j(\tau))([z_{j+1}](\tau) - \tilde{v}_j(\tau)) + \\
& q(\tau, [u_1](\tau), [v_j](\tau) - \tilde{v}_j(\tau)) \Big)\, d\tau \quad \text{with } \tilde{v}_j(t) \in [v_j](t),
\end{aligned}$$

$$[u_{j+1}](t) := [z_{j+1}](t) \cap [v_j](t).$$

(q is defined in (17).) Bauch proves the local quadratic convergence in [12]. However, in each step one has to solve a system of linear differential equations. If one uses a

(linear convergent) Picard iteration for this problem, the quadratic convergence of Newton's iteration becomes meaningless. However, one can solve particular linear problems explicitly.

A linear initial value problem

$$v' = A(t)v + g(t), \quad v(t_0) = v_0 \in V_n(\mathbf{R})$$

with $A \in C([t_0, t_1], M_{nn}(\mathbf{R}))$ and $g \in C([t_0, t_1], V_n(\mathbf{R}))$ has the unique solution

$$v^*(t) = X(t)v_0 + X(t) \int_{t_0}^{t} X^{-1}(\tau)\, g(\tau)\, d\tau, \quad t \in [t_0, t_1],$$

where $X(t)$ is the solution of the matrix initial value problem

$$X' = A(t)X, \quad X(t_0) = I.$$

$X(t)$ is called the *matricant* of the system. It exists and is regular for all $t \in [t_0, t_1]$ (see eg Gantmacher [25]). For a constant matrix A, we have

$$X(t) = \exp(A \cdot (t - t_0)).$$

We only have to compute a matrix exponential in order to evaluate it. For $n = 1$ we have

$$X(t) = \exp(\int_{t_0}^{t} A(\tau)\, d\tau).$$

In this case we can enclose $v^*(t)$ using interval integration and a "continuous interval evaluation" of the exponential function.

In 1919, Chaplygin [15] bounds the solution of scalar differential equations by solving the linear differential equations

$$\begin{aligned} \underline{u}'_{j+1} &= f(t, \underline{u}_j(t)) + \frac{f(t, \overline{u}_j(t)) - f(t, \underline{u}_j(t))}{\overline{u}_j(t) - \underline{u}_j(t)} (\underline{u}_{j+1} - \underline{u}_j(t)), \\ \overline{u}'_{j+1} &= f(t, \underline{u}_j(t)) + \frac{\partial f}{\partial u}(t, \underline{u}_j(t))(\overline{u}_{j+1} - \underline{u}_j(t)) \end{aligned}$$

(see also [53]). He obtains convergent sequences of lower and upper bounds provided that $\frac{\partial^2 f}{\partial u^2}(t, u) < 0$ holds in a certain domain.

In 1981, Raith [66] presents a Newton-like method for systems which only requires the solution of scalar linear differential equations. It is particularly mentioned in Nickel's review [62]. In a basic step, Raith generates two line segments $\underline{u}_1(t)$ and $\overline{u}_1(t)$ as a lower and an upper function, respectively. He improves the bounds iteratively by

$$\underline{u}_{j+1}(t) := \underline{u}_j(t) + \underline{v}_{j+1}(t),$$

$$\overline{u}_{j+1}(t) := \overline{u}_j(t) - \overline{v}_{j+1}(t).$$

The functions $\underline{v}_{j+1}(t)$ and $\overline{v}_{j+1}(t)$ are the solutions of the linear initial value problems

$$\overline{v}'_{j+1} + D_L \overline{v}_{j+1} = \overline{u}'_j(t) - f(t, \overline{u}_j(t)) - (L - D_L)(\overline{u}_j(t) - \underline{u}_j(t)), \tag{18}$$

$$\overline{v}_{j+1}(t_0) = 0$$

and

$$\underline{v}'_{j+1} + D_L \underline{v}_{j+1} = f(t, \underline{u}_j(t)) - \underline{u}'_j(t) - (L - D_L)(\overline{u}_j(t) - \underline{u}_j(t)), \tag{19}$$

$$\underline{v}_{j+1}(t_0) = 0,$$

respectively. L denotes a Lipschitz matrix satisfying

$$|f(t,u) - f(t,v)| \leq L|u - v| \quad \text{for } t \in [t_0, t_1], v \in [u] \subseteq D$$

(with $[u_0] \subseteq [u]$ and $[u_1](t) \subseteq [u]$), and D_L is the diagonal matrix with $D_{Lii} = L_{ii}$, $i = 1, 2, \ldots, n$. The differential equations in (18) and (19) are uncoupled and fall into $2n$ scalar equations. For details see Raith [66].

We have seen several approaches for an iterative improvement of solution bounds. (Of course, one can apply the methods to problem (3) as well.) Each of them uses "continuous integration". However, the computation of (tight) continuous bounds of the integrals is very difficult if we cannot integrate the respective expressions formally. An implementation of an iterative method for the general problem (1) is not known to the author.

5. Bounding the error of a continuous approximation

In this section we outline the principle of *continuous error methods* (see Section 1). One can describe their rough structure as follows. They generate a continuously differentiable approximate solution $\tilde{u}(t)$, enclose the defect $d(t)$ of this approximation, estimate some error bounds, and verify them using an inclusion theorem of Section 3.

For the first step, one uses some classical non-interval methods. Usually, one applies a *single–step method* (eg Runge-Kutta) in order to get a pointwise approximation. After that, one produces a continuous approximation by interpolation (see eg [7, 51, 79, 87]). In this computation, round-off errors are allowed. It actually does not matter how the approximate solution is obtained. However, one has to compute its defect exactly or enclose it using interval arithmetic.

An approximation $\tilde{u}(t)$ of $u^*(t)$ is the exact solution to a neighbouring problem. One can interpret the defect of $\tilde{u}(t)$ as a measure for the distance of this problem from the specified problem (1). In this sense, Corless and Corliss [19] bound the "error in the problem" by bounding the defect. However, this approach is different from our intention. We consider the fixed problem (1) and want to bound the error of $\tilde{u}(t)$. The results of Section 3 applied to the error problem (3) enable us to do this.

If we inflate the initial error inclusion $[e_0] := [u_0] - \tilde{u}(t_0)$ and vary the stepsize $h = t_1 - t_0$, we can always fulfil the corresponding inclusion conditions of 3.2, 3.3, or 3.4, for instance.

Let $[e]$ be an inflation of $[e_0]$ with $\tilde{u}(t) + [e] \subseteq D$ on $[t_0, t_1]$, and

$$g(t,e) := f(t, \tilde{u}(t) + e) - f(t, \tilde{u}(t)) + d(t) \quad (= f(t, \tilde{u}(t) + e) - \tilde{u}'(t)).$$

Then one can compute the range $[g]$ of $g(t,e)$ for $t \in [t_0, t_1], e \in [e]$ (or at least an inclusion of it) and a real number $s \in (t_0, t_1]$ with

$$[\hat{e}](t) := [e_0] + (t - t_0)[g] \subseteq [e]$$

for $t \in [t_0, s]$ (cf (8)). According to Theorem 3.3, $e(t) \in [\hat{e}](t)$ holds for $t \in [t_0, s]$.

We could apply this method to the original problem (1) as well. However, a linear inclusion of $u^*(t)$ cannot be tight if the derivative of $u^*(t)$ changes fast. In contrast, a linear error inclusion $[\hat{e}](t)$ can be arbitrarily tight if $\tilde{u}(t)$ is sufficiently close to $u^*(t)$. Nevertheless, this simple strategy seldom yields satisfying results. A pure inflation of $[e_0]$ does not regard any property of the specified problem, and it often restricts the stepsize $s - t_0$ too much.

Some other approaches are based on a *linearization* of the problem. One can transform the error equation in (3) into a system of linear differential equations

$$e' = L(t)e + d(t), \tag{20}$$

where the elements $L_{ij}(t)$ of the matrix $L(t)$ are the partial derivatives $\dfrac{\partial f_{(i)}}{\partial u_{(j)}}(t, u)$ of f evaluated at particular "points" $u_k^{ij}(t)$ between $u^*_{(k)}(t)$ and $\tilde{u}_{(k)}(t)$, $k = 1, 2, \ldots, n$ (see eg Hunger [32], Bauch [10]). Hunger [31, 32] uses a polynomial *a priori* inclusion of $u^*(t)$ and computes continuous bounds of $L(t)$. Following an idea of Hellman [29], he encloses the *matricant* of (20) (see Section 4) using a particular partition of $L(t)$. Interval integration leads to an inclusion of $e(t)$, finally. However, there is no implementation of this method. It is not suitable for automatic computation.

Other choices of $L(t)$ are possible as well. Uhlmann [87] estimates the so-called *Lipschitz quotients*

$$\begin{aligned} L_{ij}(t) \;=\; & \big(f_{(i)}(t, \tilde{u}_{(1)}(t), \tilde{u}_{(2)}(t), \ldots, \tilde{u}_{(j-1)}(t), u^*_{(j)}(t), u^*_{(j+1)}(t), \ldots, u^*_{(n)}(t)) - \\ & f_{(i)}(t, \tilde{u}_{(1)}(t), \tilde{u}_{(2)}(t), \ldots, \tilde{u}_{(j-1)}(t), \tilde{u}_{(j)}(t), u^*_{(j+1)}(t), \ldots, u^*_{(n)}(t))\big) : \\ & (u^*_{(j)}(t) - \tilde{u}_{(j)}(t)) \end{aligned}$$

by constant bounds.

One can find an upper bound of $|e(t)|$ with the help of Corollary 3.8.

Example 1 *We consider the scalar model problem*

$$u' = -u^2, \quad u(1) = 1 \tag{21}$$

with the solution

$$u^*(t) = \frac{1}{t}, \quad t \geq 1.$$

Even if u^* was not known, one could easily see that

$$u^*(t) \in [0, 1] =: [u] \quad \textit{for} \quad t \geq 1$$

since u is decreasing ($f(t, u) \leq 0$), and $u(t) \equiv 0$ is a solution of $u' = -u^2$.

With $\tilde{u}(t) \equiv 1$ we get $d(t) = -1$ and

$$|d(t)| = 1 =: h(t).$$

From $\dfrac{\partial f}{\partial u} = -2u$ it follows that $L(t) \in [-2, 0]$, and hence

$$L(t) \leq 0 =: K(t).$$

The solution of

$$v' = K(t)v + h(t) = 1, \quad v(t_0) = e(t_0) = 0$$

is $v(t) = t - 1$. *Due to Corollary* 3.8, *we obtain*

$$u^*(t) \in [\tilde{u}(t) - v(t), \tilde{u}(t) + v(t)] = [2 - t, t].$$

Intersection of this interval with $[u]$ *finally yields*

$$u^*(t) \in \begin{cases} [2-t, 1], & t \in [1, 2] \\ [0, 1], & t > 2 \end{cases}.$$

Sometimes one can obtain better results (for $n > 1$) by performing a linear transformation

$$e(t) = Av(t)$$

with a regular matrix $A \in M_{nn}(\mathbf{R})$ (see Uhlmann [87]). Then (20) changes into

$$v' = \tilde{L}(t)v + \tilde{d}(t)$$

with $\tilde{L}(t) = A^{-1}L(t)A$ and $\tilde{d}(t) = A^{-1}d(t)$. If $w(t)$ is an upper bound of $|v(t)|$, then we have

$$|e(t)| \leq |A|w(t).$$

However, the estimation of $L(t)$ or $\tilde{L}(t)$ by constant bounds seldom yields tight error bounds. Let us turn to a more sophisticated approach.

The most famous *continuous error method* is the method of Marcowitz presented in [51] (and emphasized in [60, 85] and others). It is based on a method of Schröder who has evolved it for a single differential equation ($n = 1$), originally (see Schröder [78, 79]). Marcowitz uses some monotone and quasimonotone decompositions for the case $n > 1$. He does not use interval arithmetic yet. However, Conradt [18] presents an interval version of Marcowitz' method in 1980 and implements it for particular problems using interval arithmetic. The method is based on an inclusion theorem that follows from Theorem 3.7 applied to the error problem (3). As Conradt, we use interval notation.

Theorem 5.1 (see Marcowitz [51], Conradt [18]) *Let* $\tilde{u}(t)$ *be a continuously differentiable approximation of* $u^*(t)$ *with* $\tilde{u}(t) \in D$ *for* $t \in [t_0, t_1]$, *and let* $d(t)$ *be its defect. Let the matrix* $\dfrac{\partial f}{\partial u}(t, \tilde{u}(t))$ *be decomposed as follows:*

$$\frac{\partial f}{\partial u}(t, \tilde{u}(t)) = D^+(t) - D^-(t) + R(t),$$

where $D^+(t)$ *and* $D^-(t)$ *are nonnegative diagonal matrices, and* $R_{ii}(t) \equiv 0$ *for* $t \in [t_0, t_1]$, $i = 1, 2, \ldots, n$. *Let* $[m](z)$ *be an interval function satisfying*

$$f(t, \tilde{u}(t) + z) - f(t, \tilde{u}(t)) - \frac{\partial f}{\partial u}(t, \tilde{u}(t))z \in [m](z)$$

for $t \in [t_0, t_1]$ and $\tilde{u}(t) + z \in D$. If an interval function $[v](t)$ with continuously differentiable bounds $\underline{v}(t)$ and $\overline{v}(t)$ exists satisfying

$$u_0 - \tilde{u}(t_0) \in [v](t_0), \quad \tilde{u}(t) + [v](t) \subseteq D,$$

and

$$[\underline{v}'(t) + D^-(t)\underline{v}(t), \overline{v}'(t) + D^-(t)\overline{v}(t)] \supseteq d(t) + (D^+(t) + R(t))[v](t) + [m]([v](t))$$

for $t \in [t_0, t_1]$, then the inclusion

$$e(t) \in [v(t)]$$

holds on this interval.

Remark: One can validate bounds $\underline{v}(t), \overline{v}(t)$ with $\underline{v}'(t) \geq \overline{v}'(t)$ provided that $D^-(t)$ does not vanish. However, if the diagonal of $\dfrac{\partial f}{\partial u}$ has no negative elements, Theorem 5.1 has no advantage over Corollary 3.5. In this case, the width of the inclusion always increases with t.

Marcowitz and Conradt solve some particular linear differential inequalities in order to get two functions $\underline{v}(t)$ and $\overline{v}(t)$ satisfying the conditions of 5.1. They first ignore the nonlinear term $[m]$ and then estimate it by linear terms. For details see Marcowitz [51]. Numerical results are shown in [51] and [18]. The error bounds sometimes have the same sign, i.e. some components of the error inclusion $[e](t)$ do not contain the number zero. In this case, the inclusion $[u](t) = \tilde{u}(t) + [e](t)$ does not contain the approximate solution $\tilde{u}(t)$.

In contrast, the original method of Schröder generates an upper bound $z(t) \geq 0$ of the absolute value of the error. We get the inclusion

$$u^*(t) \in [u](t) = \tilde{u}(t) + [-z(t), z(t)]$$

which always contains $\tilde{u}(t)$. The same holds for methods which apply Corollary 3.8 to a linearized problem (see Example 1). The error estimation cannot be better than the approximate solution.

Marcowitz' method yields tight bounds in particular problems. However, a program for the automatic solution of the general problem (1) does not exist yet. The method consists of many different procedures. The complete description (see Marcowitz [51]) is too extensive to be set out here.

A continuous error method does not necessarily have to use the defect or the derivative of the approximate solution $\tilde{u}(t)$. One can perform one step of the Picard-Lindelöf iteration (4) with $u_1(t) := \tilde{u}(t)$ instead. Theorem 3.1 (or a similar inclusion theorem) yields bounds of the error of $u_2(t)$. However, in this case one must compute $u_2(t)$ without any round-off error. In digital computation, one has to use interval integration in order to get an inclusion of $u_2(t)$.

6. Bounding the truncation error of a single-step method

The difficulty in the methods mentioned in Section 4 and Section 5 is the necessity to differentiate or to integrate continuous functions and to represent them on an interval $[t_0, t_1]$. We now follow a quite different approach. We only use function evaluations instead of function expressions. The idea goes back to Moore [52].

The methods of Section 5 use a continuous approximate solution which may be obtained by an arbitrary non-interval method. In contrast, we now consider a particular method and use some of its properties in order to enclose the error.

The simplest classical methods are the *single-step methods* (Runge-Kutta or Taylor series). They compute pointwise approximations $\tilde{u}_j$ of $u^*(t)$ on a grid $\{t_1, t_2, \ldots, t_m\}$ $(j = 1, 2, \ldots, m)$. *Discrete error methods* estimate their truncation errors and yield a sequence $\{[u_j]\}_{j=1}^{m_0}$ of interval vectors with $u^*(t_j) \in [u_j]$ for $j = 1, 2, \ldots, m_0,\ m_0 \leq m$. An exception is given by Collatz [16] and Schmidt [77]. They compute error bounds of the global error of Euler's method *a posteriori*.

In approximate computation, the *Runge-Kutta methods* are usually prefered to the *Taylor series method* since they do not require the derivatives of f. However, the Taylor method has a decisive advantage for enclosure methods because its *local truncation error* can be estimated very simply. Therefore, interval Runge–Kutta methods appear very seldom. (Oelschlägel *et al.* [63, 64] and Shokin [82] show some examples.) Moreover, Corliss remarks in [20] that interval Taylor methods mostly yield tighter bounds. The Taylor polynomial is evaluated at a single point. Runge-Kutta methods (as well as multi-step methods) use combinations of function values at different points. If we replace every real value by an interval, we have to evaluate interval sums. However, in interval arithmetic one tries to avoid sums since the width of a sum is equal to the sum of the widths.

In the following, we only pursue the Taylor approach. For the moment, we consider a single step from t_0 to t_1 with the stepsize $h := t_1 - t_0$. We assume that f is p times differentiable ($p \in \mathbf{N}$). This is a new assumption which seems to be very restrictive. However, we only use combinations of standard functions for computing, usually. They are analytic (at least piecewise) in their domain. Hence, our requirement is not very restrictive in practice.

We can write the solution u^* of (1) at t_1 in the form

$$u^*(t_1) = u_0 + \sum_{k=1}^{p} h^k f^{(k)}(t_0, u_0) + h^{p+1}\hat{u} \tag{22}$$

with

$$f^{(1)} = f, \quad f^{(k+1)} = \frac{1}{k+1}\left(\frac{\partial f^{(k)}}{\partial t} + \frac{\partial f^{(k)}}{\partial u} f\right),$$

and

$$\hat{u}_{(i)} = f_{(i)}^{(p+1)}(\tau_i, u^*(\tau_i))$$

for particular values $\tau_i \in [t_0, t_1]$, $i = 1, 2, \ldots, n$. $f^{(k)}(t, u^*(t))$ is the k-th *Taylor coefficient* of $u^*(t)$:

$$f^{(k)}(t, u^*(t)) = \frac{1}{k!}\frac{d^k u^*}{dt^k}(t).$$

Moore [52, 54, 55] and Lohner [47] give rules for the automatic evaluation of these coefficients on a computer. They are based on *automatic differentiation* (see eg Rall [67–69]). Using the known differentiation rules, one can evaluate the derivatives of functions with a finite representation without any symbolic differentiation.

For example, let $v(t)$ and $w(t)$ be two q-times differentiable functions whose Taylor coefficients at a point s are known:

$$v_k := \frac{1}{k!}\frac{d^k v}{dt^k}(s), \quad w_k := \frac{1}{k!}\frac{d^k w}{dt^k}(s), \quad k = 0, 1, \ldots, q.$$

Then the k-th Taylor coefficient of the product of $v(t)$ and $w(t)$ is given by

$$(v \cdot w)_k := \frac{1}{k!}\frac{d^k(v \cdot w)}{dt^k}(s) = \sum_{j=0}^{k} v_j w_{k-j}. \tag{23}$$

One can apply these methods and evaluate the Taylor coefficients of u^* at s successively if only $u^*(s)$ is known. Due to the relation $u^{*'}(t) = f(t, u^*(t))$, the k-th Taylor coefficient of u^* yields the k-th coefficient of $f(= u^{*'})$ and hence the $(k+1)$-st coefficient of u^*.

Example 2 *We consider problem* (21) (see Example 1, Section 5). *The k-th Taylor coefficient of $u^{*'}(t)$ at t_0 is*

$$(k+1) f^{(k+1)}(t_0, u_0) =: (k+1) f^{(k+1)}.$$

It follows from (23) *that*

$$f^{(k+1)} = -\frac{1}{k+1}\sum_{j=0}^{k} f^{(j)} f^{(k-j)} \quad (f^{(0)} := u_0).$$

With $u_0 = 1$ we obtain

$$f^{(k)} = (-1)^k,$$

and hence

$$u^*(t_0 + h) = \sum_{k=0}^{\infty}(-h)^k \quad (\textit{for } h < 1).$$

The Taylor series method uses formula (22) (without the *remainder term* $h^{p+1}\hat{u}$). One obtains an inclusion of the solution by enclosing the remainder term. This approach is known as *Moore's method*. Moore describes it in [52]. Assume that $[\hat{u}]$ is a constant inclusion of $u^*(t)$ on the interval $[t_0, t_1]$ (produced by Algorithm 1 in Section 3, for instance). Then Moore's method generates the interval vector

$$[u_1] = [u_0] + \sum_{k=1}^{p} h^k f^{(k)}(t_0, [u_0]) + [z_1] \tag{24}$$

with

$$[z_1] = h^{p+1}\, f^{(p+1)}([t_0, t_1], [\hat{u}]).$$

Due to equation (22), we have

$$u^*(t_1) \in [u_1]$$

since $[z_1]$ contains the local truncation error $h^{p+1}\hat{u}$ of the classical Taylor series method.

Theoretically, we can compute arbitrarily sharp enclosures by increasing the integer p if $[u_0] = u_0$ (i.e. $w([u_0]) = 0$) and if h is small enough (see Example 2).

Example 2 (continued) *We take the constant inclusion* $[\hat{u}] = [0,1]$ *from Example* 1 *and get*

$$[z_1] = (-h)^{p+1}[0,1].$$

The width of the error inclusion converges to 0 *for* $p \to \infty$ *if* $h < 1$.

With $p = 2$ *and* $t_1 = 1.5$ *(i.e.* $h = 0.5$*), we get*

$$[u_1] = 1 - \frac{1}{2} + \frac{1}{4} - \frac{1}{8}[0,1] = [0.625, 0.75].$$

Apart from the simple representation for the truncation error, the Taylor series method has some further advantages. One can easily change the order by increasing or decreasing p, i.e. by adding or deleting some terms in the right hand side of (24) and adapting the remainder. One can change the stepsize without computing new Taylor coefficients. If we let h vary, we get a continuous inclusion in the form of an interval polynomial. Moreover, the method can efficiently be implemented on a computer by using automatic differentiation.

If we have computed an inclusion $[u_1]$ of the solution $u^*(t_1)$, we can improve the constant inclusion on $[t_0, t_1]$ *a posteriori* by

$$[\hat{u}]_{new} := [\hat{u}] \cap \Big([u_0] + [0,h]\, f([t_0,t_1],[\hat{u}])\Big) \cap \Big([u_1] - [0,h]\, f([t_0,t_1],[\hat{u}])\Big).$$

Using this new interval vector, we can improve the inclusion of the remainder and the solution as well (see eg Lohner [47]).

Example 2 (continued)

$$\begin{aligned}[\hat{u}]_{new} &= [0,1] \cap (1 + [0,0.5][-1,0]) \cap ([0.625, 0.75] - [0,0.5][-1,0]) \\ &= [0,1] \cap [0.5,1] \cap [0.625, 1.25] = [0.625, 1].\end{aligned}$$

$$[u_1]_{new} = 1 - \frac{1}{2} + \frac{1}{4} - \frac{1}{8}[0.625, 1] = [0.625, 0.671875].$$

This procedure can be iterated. However, in practice one mostly performs one single step only. A second step seldom improves the result noticeably. (In Example 2, a second iteration step yields the same inclusion.)

Of course, one can also use other methods to improve $[\hat{u}]$. Krückeberg [41] suggests a Picard-Lindelöf iteration, for instance. In the following, we always assume that we know a constant inclusion (which may already be improved), and that we have already computed the error inclusion $[z_1]$.

Remark: A much bigger problem than the width of the constant inclusion is its domain. Unfortunately, the requirement (7) in Corollary 3.4 strongly restricts the choice of the stepsize h. h has to be as small as a suitable stepsize for Euler's method, approximately, in order to fulfil (7) (see eg Lohner [47], Stetter [85]). Stetter shows in [85] that an interval vector $[\hat{u}]$ satisfying (7) with a certain h_0 is often *inclusion valid* for much bigger steps than h_0. That means,

$$e(t_0 + h) \in [z](h) := h^{p+1} f^{(p+1)}([t_0, t_0 + h], [\hat{u}])$$

even holds for some $h > h_0$. He gives some results for linear systems. Lohner has recently generalized Stetter's results for nonlinear problems in [49]. He uses an interval polynomial arithmetic to verify *a priori* error bounds on large intervals. However, his method has not been implemented yet.

Moore evaluates the expression

$$\psi(t, [u]) := [u] + \sum_{k=1}^{p} h^k f^{(k)}(t, [u])$$

directly. That means, he replaces the variable u in the function $\psi(t, u)$ by an interval $[u]$ and performs all operations in interval arithmetic. This method is width-increasing, i.e.

$$w([u_1]) = w(\psi(t_0, [u_0])) + w([z_1]) \geq w([u_0]).$$

Alefeld and Herzberger show in [5] that the *mean-value evaluation* often yields tighter inclusions than the *direct evaluation* (see also Neumaier [57]). Therefore, we replace $\psi(t, [u])$ by the *mean-value form*

$$\psi(t, \tilde{u}) + \frac{\partial \psi}{\partial u}(t, [u])\,([u] - \tilde{u}), \quad \tilde{u} \in [u]$$

(see [73]).

The matrices $\dfrac{\partial \psi}{\partial u}$ also appear in the methods of Eijgenraam [23] and Lohner [47] which are described in Section 8. Lohner shows in [47] that one can compute $\dfrac{\partial \psi}{\partial u}(t, [u])$ using automatic differentiation if only a finite representation of $\dfrac{\partial f}{\partial u}(t, u)$ is given.

In contrast to Moore's method, the *mean-value method* can be width-decreasing. That means, the inclusion

$$[u_1] = \psi(t_0, \tilde{u}_0) + \frac{\partial \psi}{\partial u}(t_0, [u_0])\,([u_0] - \tilde{u}_0) + [z_1], \quad \tilde{u}_0 \in [u_0]$$

can have a smaller width than $[u_0]$. This can happen if the inclusion $[z_1]$ of the truncation error is sufficiently tight, and if the diagonal elements of $\dfrac{\partial f}{\partial u}$ are negative (see [73]) (cf the remark after Theorem 5.1).

Example 3 *We consider the differential equation*

$$u' = -c\,u$$

with a positive constant c. With $p = 1$, Moore's method yields

$$[u_1] = [u_0] + hf(t_0, [u_0]) + [z_1] = [u_0] - ch[u_0] + [z_1]$$

and

$$w([u_1]) = (1 + c\,h)\,w([u_0]) + w([z_1]) > w([u_0]) \quad \textit{for} \quad h > 0.$$

The mean-value method leads to the inclusion

$$\begin{aligned}[u_1] &= \tilde{u}_0 + hf(t_0, \tilde{u}_0) + (1 + h\frac{\partial f}{\partial u}(t_0, [u_0]))([u_0] - \tilde{u}_0) + [z_1] \\ &= \tilde{u}_0 - ch\tilde{u}_0 + (1 - ch)([u_0] - \tilde{u}_0) + [z_1]\end{aligned}$$

and to the width

$$w([u_1]) = |1 - c\,h|\,w([u_0]) + w([z_1]).$$

For some h, the method is width-decreasing if $w([u_0]) > 0$ and if $w([z_1])$ is small enough.

However, both methods yield the same results if $w([u_0]) = 0$.

Krückeberg [41], Eijgenraam [23], and Lohner [46] take on the basic idea of Moore and present modified methods which take the *wrapping effect* into account. We will discuss this effect in Section 7. It does not affect a single integration step (from t_0 to t_1).

Mannshardt [50] describes a method which differs from other approaches since it does not use interval arithmetic. He computes the lower and upper bounds using different stepsizes in general. This is useful in the case of differential equations with singularities or discontinuities. However, it only handles scalar equations.

7. The wrapping effect, particular problems

Up to now, we have considered the enclosure of $u^*(t)$ at a single grid point or a single interval (bounded by two grid points) only. However, we want to enclose the solution on the whole grid $\{t_0, t_1, \ldots, t_m\}$ and have to perform our method m times (at least). With an inclusion $[u_j]$ of $u^*(t_j)$, we get a new initial condition

$$u(t_j) \in [u_j]$$

in the $j + 1$-st step.

In general, the inclusion $[u_j]$ of $u^*(t_j)$ contains "false" solutions, i.e. solutions $\hat{u}(t)$ of the differential equation $u' = f(t, u)$ with $\hat{u}(t_{j-1}) \notin [u_{j-1}]$ or solutions which do not even exist at t_{j-1}. At t_{j+1} new false solutions are caught, and so forth (see Picture 1).

The use of interval arithmetic leads to an additional effect known as the *wrapping effect*. In general, the set

$$\{u(t_j; t_{j-1}, [u_{j-1}])\} \tag{25}$$

(see Section 2) is not an interval (a rectangle with sides parallel to the coordinate axes in the case of $n = 2$), but it is wrapped by an interval $[u_j]$. This process can lead to immense overestimations even if one has the interval hull, i.e. the closest interval including the set (25). Moore shows a very simple example in [53] and [54]:

The solutions of $u' = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} u$ are circles in the (u_1, u_2)–phase space. The set (25) is a rotated rectangle whose interval hull $[u_j]$ is wider than $[u_{j-1}]$. One rotates and wraps this interval hull anew and gets an interval vector $[u_{j+1}]$ that is not even the hull of $\{u(t_{j+1}; t_{j-1}, [u_{j-1}])\}$ in general. All points of this set may lie in the interior of $[u_{j+1}]$ even if we use exact interval arithmetic (see Picture 2). Moore shows that the widths of the inclusions grow exponentially, even if the stepsize converges to zero (see [53, 54]). However, the actual set of solutions does not increase.

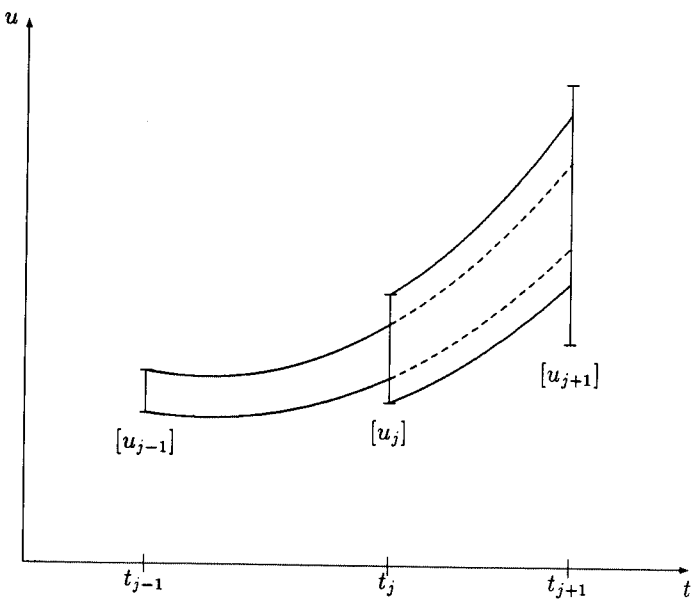
This simple example impressively shows the obstacles appearing in interval arithmetic algorithms. Various attempts have been made to overcome these difficulties. In [53] and [54], Moore compensates for the rotation in the above example with a *local coordinate transformation*. His "intervals" do not have to be parallel to the original coordinate axes of the phase space. He works with *parallelepipeds*. One can write a parallelepiped as a pair of a real matrix and an interval vector defined by

$$(A, [u]) := \{A\, u \mid u \in [u]\}.$$

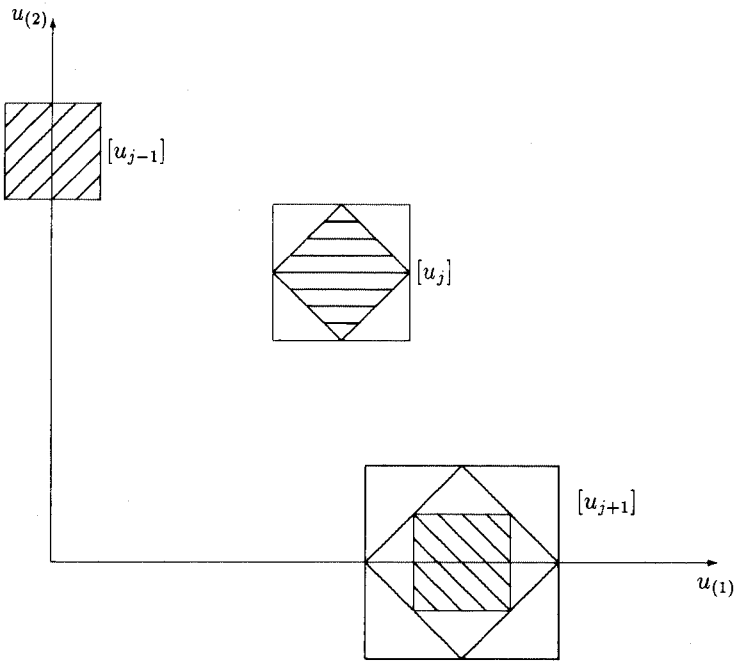
This set is contained in the interval product $A[u]$. However, Jackson showed in [34] that Moore's coordinate transformation can lead to catastrophic overestimations in other examples.

Stewart and Davey use polyhedrons as enclosure sets (see [22] and [86]). Kahan [35] and several other authors use ellipsoids (see eg [27, 28, 33, 43]). Each of these methods is able to avoid the wrapping effect in some particular problems.

Picture 1



Picture 2



Independently of each other, Lohner [45] and Nickel [58] evolved another approach for systems of *linear* differential equations. They consider the initial value problem

$$u'(t) = A(t)\,u(t) + g(t), \quad u(t_0) = u_0 \tag{26}$$

with A and g continuous in $[t_0, T]$. The unique solution of (26) is

$$u^*(t) = X(t)\,u_0 + X(t) \int_{t_0}^{t} X^{-1}(\tau)\,g(\tau)\,d\tau, \tag{27}$$

where $X(t)$ is the *matricant* of the system (see Section 4).

Obviously, (27) describes an affine transformation of u_0 for fixed t. If we replace u_0 by a parallelepiped $(Y, [u_0])$ with $Y \in M_{nn}(\mathbb{R})$, then the result of this transformation is a parallelepiped whose corners are the image points of the corners of $(Y, [u_0])$. Since a parallelepiped is determined by $n+1$ corners, one obtains an exact representation of the solution set by solving $n+1$ systems of n linear differential equations with real vectors as initial values (see [45, 58, 61]). In contrast, an interval evaluation of (27) with an initial interval $[u_0]$ generally leads to an overestimation. In practice, however, one obtains interval inclusions of the $n+1$ corners instead of the exact points. A new difficulty has to be overcome in order to continue the method. One has to determine the corners of a nearby parallelepiped which contains those $n+1$ interval vectors. Conradt solves this problem in [18] for $n = 2$.

Bauch and Kimmel [14] point out that these methods can be connected to Newton iteration methods. We have seen in Section 4 that every Newton step contains the problem of solving a system of linear differential equations.

Another class of particular problems (besides the linear differential equations) are the *quasimonotone* systems introduced in Section 3. We have seen that the solution set in Moore's example may not even have a single common point with the boundary of the interval inclusion after only two steps. This is not the case if f is quasimonotone. Using Theorem 3.6, one can easily prove

Theorem 7.1 (see also Nickel [59, 60] and Oelschlägel, Wiebigke [65]) *Let $f(t,u)$ be quasimonotone in u, $[u_0] \subseteq D$. Assume that $\underline{u}(t)$ is the solution of $u' = f, u(t_0) = \underline{u}_0$, and that $\overline{u}(t)$ is the solution of $u' = f, u(t_0) = \overline{u}_0$. Then the inclusion*

$$\{u(t)\} := \{u(t; t_0, [u_0])\} \subseteq [\underline{u}(t), \overline{u}(t)]$$

holds.

Hence, one can determine the interval hull of $\{u(t)\}$, and the interval bounds belong to $\{u(t)\}$. Even if the set $\{u(t_j; t_{j-1}, [u_{j-1}])\}$ is wrapped by its interval hull $[u_j]$ again and again at the grid points t_j $(j = 1, 2, \ldots, m)$, the bounds remain the same, i.e.

$$\underline{u}_j = \underline{u}(t_j) \quad \text{and} \quad \overline{u}_j = \overline{u}(t_j).$$

Of course, we cannot wrap these sets by their hulls in practice. We overestimate them in every step since we cannot solve the initial value problems exactly.

If f is quasimonotone, we can divide the problem

$$u' = f(t,u), \quad u(t_j) \in [u_j] \tag{28}$$

into two problems with the "real" initial conditions

$$u(t_j) = \underline{u}_j \quad \text{and} \quad u(t_j) = \overline{u}_j,$$

respectively. Due to Theorem 7.1, the interval hull of the two solutions includes the solution set of (28). If we use interval Taylor methods, we can avoid the computation of $\dfrac{\partial \psi}{\partial u}$ since real initial vectors do not require the mean-value method (see Section 6).

In general, however, we have to handle initial intervals and to face the wrapping effect.

8. Wrapping in Taylor methods

We want to study the wrapping effect in interval Taylor methods in order to evolve methods to reduce it. For a sequence of steps with the stepsizes $h_j = t_j - t_{j-1}$, *Moore's method* is defined recursively by

$$[u_j] = \psi_j(t_{j-1}, [u_{j-1}]) + [z_j]$$

with

$$\psi_j(t,u) := u + \sum_{k=1}^{p} h_j^k f^{(k)}(t,u)$$

and

$$[z_j] = h_j^{p+1} f^{(p+1)}([t_{j-1}, t_j], [\hat{u}_j]).$$

$[\hat{u}_j]$ denotes a constant inclusion of $u^*(t)$ on $[t_{j-1}, t_j]$.

Even if u_0 is given as a real vector, $[u_1]$ is already an interval vector with $w([u_1]) > 0$ in general. All further steps are at the mercy of the wrapping effect.

Krückeberg uses the following modification in [41]. He chooses a real vector $\tilde{u}_{j-1}$ out of $[u_{j-1}]$ and computes an inclusion of the solution $\tilde{u}(t)$ of the problem

$$u' = f(t, u), \quad u(t_{j-1}) = \tilde{u}_{j-1}$$

using Moore's method:

$$\tilde{u}(t_j) \in [\tilde{u}_j] = \psi_j(t_{j-1}, \tilde{u}_{j-1}) + [\tilde{z}_j]$$

(with an appropriate inclusion $[\tilde{z}_j]$ of the corresponding remainder term). Since the defect of $\tilde{u}(t)$ vanishes, we get the error equation

$$\begin{aligned} e' &= f(t, u^*(t)) - f(t, \tilde{u}(t)) \\ &= L(t)\, e \end{aligned} \tag{29}$$

(cf (3) and (20)) with an unknown matrix $L(t) \in \dfrac{\partial f}{\partial u}(t, [\hat{u}_j])$, where $[\hat{u}_j]$ is a constant inclusion of both $u^*(t)$ and $\tilde{u}(t)$. Thus we get

$$e(t_j) \in [Q_j]\, e(t_{j-1})$$

with

$$[Q_j] = \exp\left(h_j \frac{\partial f}{\partial u}([t_{j-1}, t_j], [\hat{u}_j]) \right)$$

and finally

$$u^*(t_j) \in [u_j] := [\tilde{u}_j] + [Q_j]\,([u_{j-1}] - \tilde{u}_{j-1}). \tag{30}$$

Krückeberg chooses parallelepipeds as inclusion sets in order to avoid the direct interval evaluation of the right hand side. That means, he uses a representation which is similar to Moore's coordinate transformation (Moore [53]). The details are set out in [41].

A similar method, which is also working with a real vector $\tilde{u}_{j-1} \in [u_{j-1}]$, is the *mean-value method* introduced in Section 6. If we abbreviate

$$[Q_j] := \frac{\partial \psi_j}{\partial u}(t_{j-1}, [u_{j-1}]) \qquad \text{and} \qquad [\tilde{u}_j] := \psi_j(t_{j-1}, \tilde{u}_{j-1}) + [z_j],$$

we obtain representation (30) again. However, the mean-value method requires no matrix exponential. Moreover, the wide intervals $[t_{j-1}, t_j]$ and $[\hat{u}_j]$ are only used for the remainder inclusion $[z_j]$. They do not appear in the matrix $[Q_j]$ as in Krückeberg's method.

If f is sufficiently smooth, we can make $w([z_j])$ small by increasing the order p of the Taylor polynomial ψ. That means, the width of $[u_j]$ mainly depends on the product $[Q_j]([u_{j-1}] - \tilde{u}_{j-1})$.

In the previous section, we have already mentioned that the interval evaluation $A[u]$ of the product of a matrix A and an interval vector $[u]$ is an overestimation of the set $\{Au \mid u \in [u]\}$ in general. Whole sequences of such products appear if we apply the mean-value method on a grid $\{t_0, t_1, \ldots, t_m\}$, successively. They are responsible for the wrapping effect.

For the sake of simplicity, let us assume that the elements of the matrices $[Q_j] =: Q_j$ are real for $j = 1, 2, \ldots, m$. (Take a system of linear differential equations, for example.) With $[v_0] := [u_0] - \tilde{u}_0$ and $[v_j] := [\tilde{u}_j] - \tilde{u}_j$ for $j = 1, 2, \ldots, m$, the mean-value method yields

$$\begin{aligned}[u_m] - \tilde{u}_m &= [v_m] + Q_m\,([u_{m-1}] - \tilde{u}_{m-1}) \\ &= [v_m] + Q_m\,[v_{m-1}] + Q_m\,Q_{m-1}\,[v_{m-2}] + \ldots + Q_m\,Q_{m-1}\ldots\,Q_1\,[v_0],\end{aligned}$$

where the summands are evaluated as follows :

$$[s_j] := (Q_m(Q_{m-1}\ldots(Q_{j+1}[v_j])\ldots)). \tag{31}$$

That means, we have $m - j$ matrix-vector products. Each of them is wrapped by an interval vector. However, it would be sufficient to compute the interval hulls

$$[h_j] := (Q_m\,Q_{m-1}\ldots\,Q_{j+1})[v_j] \tag{32}$$

of $\{Q_m\,Q_{m-1}\ldots\,Q_{j+1}\,v \mid v \in [v_j]\}$ in order to obtain an inclusion

$$u^*(t_m) - \tilde{u}_m \in [v_m] + [h_{m-1}] + [h_{m-2}] + \ldots + [h_0].$$

We have

$$w([s_j]) = |Q_m|\,|Q_{m-1}|\ldots|Q_{j+1}|\,w([v_j])$$

but

$$w([h_j]) = |Q_m\,Q_{m-1}\ldots\,Q_{j+1}|\,w([v_j]) \leq w([s_j]).$$

If $[v_j]$ is symmetric (i.e. $\tilde{u}_j = m([\tilde{u}_j])$), the corresponding estimation holds for interval matrices $[Q_k]$ $(k = j+1, j+2, \ldots, m)$ as well.

If the stepsizes are small enough and f is quasimonotone in u, then the matrices $[Q_k]$ are nonnegative, and $[s_j]$ does not differ from $[h_j]$. This fact again shows the special position of quasimonotone systems.

However, evaluation (31) usually leads to strong overestimations in other problems. One could compute the actual hulls (32) in order to avoid them. Unfortunately, this is no feasible method since the costs will grow from step to step (see also Bachmann [9]). It would be a multi-step method which always utilizes the results of all preceding steps. Gambill and Skeel [24] suggest a combination of (31) and (32) and attain a reduction of the wrapping effect in some particular examples. All the same, we limit ourselves to methods which are carrying out the same procedure in every single step and thus are comparable to the classical single-step methods in a certain sense. One can easily implement them, and the costs do not increase during the computation.

Below we show a heuristic way to evolve an appropriate modification of the mean–value method. Let us start with the first integration step.

The interval evaluation of

$$[q_1] := [Q_1]\,([u_0] - \tilde{u}_0)$$

is the basis for the wrapping effect. We can influence it by preconditioning with a regular matrix A_1^{-1}:

$$[p_1] := \left(A_1^{-1}\,[Q_1]\right)\,([u_0] - \tilde{u}_0)$$

Let $[Q_1]$ include A_1, for example. Then $A_1^{-1}[Q_1]$ includes the identity matrix, and the product $[p_1]$ hardly causes any wrapping. The parallelepiped $(A_1, [p_1]) = \{A_1 p | p \in [p_1]\}$ contains the set $\{Qu | Q \in [Q_1], u \in [u_0] - \tilde{u}_0\}$, and it often has tighter bounds than the interval evaluation $[q_1]$. In practice, we cannot compute the matrix inverse A_1^{-1} exactly in general. We have to enclose it by an interval matrix.

We have an interval representation

$$[u_1] = [\tilde{u}_1] + [q_1]$$

of an inclusion of the solution, but we try to avoid the use of the vector $[q_1]$ in the following steps whenever it is possible.

In the second step of the mean–value method, we face the interval matrix-vector product

$$[Q_2]\,([u_1] - \tilde{u}_1) = [Q_2]\,([q_1] + [\tilde{u}_1] - \tilde{u}_1).$$

In order to separate $[q_1]$, we distribute the above product and get

$$[Q_2]\,[q_1] + [Q_2]\,([\tilde{u}_1] - \tilde{u}_1)$$

(ignoring that this is actually not allowed in interval arithmetic). Finally, we replace $[q_1]$ by $(A_1, [p_1])$. We define

$$[q_2] := ([Q_2]\,A_1)\,[p_1] + [Q_2]\,([\tilde{u}_1] - \tilde{u}_1)$$

and thus avoid the explicit interval evaluation of $A_1[p_1]$. We prepare the next step defining

$$[p_2] := \left(A_2^{-1}\,([Q_2]\,A_1)\right)\,[p_1] + \left(A_2^{-1}\,[Q_2]\right)\,([\tilde{u}_1] - \tilde{u}_1)$$

with a new regular matrix A_2.

If we perform the following steps in just the same way, we obtain the *extended mean–value method*:

$$[\tilde{u}_0] := [u_0],$$

$$[p_0] := 0 \in V_n(\mathbb{R}),$$

$$A_0 := I \in M_{nn}(\mathbb{R}),$$

$$[q_j] := ([Q_j]\,A_{j-1})\,[p_{j-1}] + [Q_j]\,([\tilde{u}_{j-1}] - \tilde{u}_{j-1}),$$

$$[p_j] := \left(A_j^{-1}\left([Q_j]\,A_{j-1}\right)\right)[p_{j-1}] + \left(A_j^{-1}\,[Q_j]\right)\left([\tilde{u}_{j-1}] - \tilde{u}_{j-1}\right),$$

$$[u_j] := [\tilde{u}_j] + [q_j]$$

with $\tilde{u}_{j-1} \in [\tilde{u}_{j-1}]$. We obtain the tightest intervals if $\tilde{u}_{j-1}$ is the midpoint $m([\tilde{u}_{j-1}])$ of $[\tilde{u}_{j-1}]$.

The results $[u_j]$ actually include the values $u^*(t_j)$ for an arbitrary choice of the matrices $A_1, A_2, \ldots$ (which have to be regular, of course). The proof is shown in [73]. However, the choice of these matrices is important for the quality of the inclusions (i.e. their widths).

The methods of Eijgenraam [23] and Lohner [47] look similar. The following algorithm shows a generalization of Eijgenraam's method (see also [73]).

$$[x_0] := [u_0],$$

$$A_0 := I \in M_{nn}(\mathbb{R}),$$

$$A_j := S_j\,A_{j-1},$$

$$[c_j] := [\tilde{u}_j] - S_j\,\tilde{u}_{j-1} + ([Q_j] - S_j)\,([u_{j-1}] - \tilde{u}_{j-1}),$$

$$[x_j] := x_{j-1} + A_j^{-1}\,[c_j],$$

$$[u_j] := A_j\,[x_j]$$

with $\tilde{u}_{j-1} \in [u_{j-1}]$.

Eijgenraam prescribes special matrices A_j in his original method (see [23]). It is the predecessor of Lohner's method which is given below.

$$[\tilde{u}_0] := [u_0],$$

$$[r_0] := [u_0] - \tilde{u}_0,$$

$$A_0 := I \in M_{nn}(\mathbb{R}),$$

$$[u_j] := ([Q_j]\,A_{j-1})[r_{j-1}] + [\tilde{u}_j],$$

$$[r_j] := \left(A_j^{-1}\left([Q_j]\,A_{j-1}\right)\right)[r_{j-1}] + A_j^{-1}\left([\tilde{u}_j] - \tilde{u}_j\right)$$

with $\tilde{u}_j \in [\tilde{u}_j]$.

Assume that we choose the same matrices A_j in each of these three methods (i.e. $S_j := A_j\,A_{j-1}^{-1}$ in Eijgenraam's method). Let $\tilde{u}_j$ always be the midpoint of $[\tilde{u}_j]$ (or $[u_j]$ in Eijgenraam's method). We assume that we perform m steps of each method on the same grid with the same error inclusions $[z_j]$, the same initial interval $[u_0]$, and the same order p of the Taylor polynomial. Let $[u_j]_M$ be the results of the extended mean-value method, $[u_j]_L$ those of Lohner's method, and $[u_j]_E$ those of Eijgenraam's method. Then we have

$$[u_j]_M \subseteq [u_j]_L \subseteq [u_j]_E \quad \text{and} \quad m([u_j]_M) = m([u_j]_L) = m([u_j]_E) \quad \text{for} \quad j = 1, 2, \ldots, m.$$

This is shown in [73].

With $A_j = I, j = 1, 2, \ldots$, the extended mean-value method and Lohner's method both turn into the ordinary mean-value method provided that $\tilde{u}_{j-1} = m([\tilde{u}_{j-1}])$ in each step (see [73]).

We try to avoid an overestimation in the matrix-vector products

$$\left(A_j^{-1}\left([Q_j]\, A_{j-1}\right)\right)[p_{j-1}] \quad \text{and} \quad \left(A_j^{-1}\left([Q_j]\, A_{j-1}\right)\right)[r_{j-1}],$$

respectively, by choosing

$$A_j = m([Q_j]\, A_{j-1}).$$

In Eijgenraam's original method, we have $S_j = m([Q_j])$ and thus get the same matrices A_j. One expects that this strategy yields the tightest inclusions since the interval matrices $A_j^{-1}([Q_j]A_{j-1})$ and $[Q_j]-S_j$ are inclusions of the identity matrix. However, Lohner showed in [47] that the condition of A_j can grow from step to step and cause a wrapping effect anew. The same difficulties appear in the predecessors of our methods namely Moore's coordinate transformation and Krückeberg's method as shown by Jackson in [34].

Actually, the above choice of A_j yields very good results in Moore's example of Section 7 (see [47]), but it leads to a catastrophic explosion of the intervals in the example

$$u' = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} u$$

(see [73, 74]). The ordinary mean-value method ($A_j = I$) is rather more suitable in this case. (The right hand side of the above equation is quasimonotone.) Of course, these effects appear in nonlinear and larger systems as well.

In general, we do not know the optimal matrices A_j. An optimal choice is not possible. However, the *QR-factorization* of Lohner is a promising method. He takes $A_j = Q$ with

$$QR = m([Q_j]\, A_{j-1})$$

where Q is an orthogonal and R an upper triangular matrix. Here the condition number of the matrices A_j cannot grow. The QR-factorization works well in both test examples.

9. Some final remarks

The interval Taylor series methods and their modifications are especially suitable for automatic computation on digital computers (see also Stetter [85]).

Lohner's method is the most popular one. His computer program AWA is printed in [47]. Besides standard inclusions, it can also generate *inner bounds*, i.e. intervals which are contained in the interval hull of the set of all solutions satisfying the initial condition $u(t_0) \in [u_0]$.

Rufeger and Adams [75] supplement the method with a *stepsize control*. Kerbl [37] uses another approach for the choice of a suitable stepsize. Both methods use an approximation of the *local excess* which is a measure of the overestimation of the solution set in each step (see eg Stetter [84]).

Wauschkuhn [92] uses Krückeberg's method to verify the existence of *periodic solutions*. Adams [1, 2] treats the same topic using Lohner's method.

In [70–73], Lohner's method is linked with other interval methods in order to enclose some *generalized solutions* of differential equations with only piecewise continuous right hand sides.

One can use a computer arithmetic with reals of variable length in order to raise the accuracy (see eg Krückeberg, Leisen [42]) or simulate such an arithmetic by using *staggered correction format* (see Lohner [48], Stetter [83]).

In [85], Stetter remarks that Lohner's program can successfully deal with a wide variety of problems. However, he also mentions that its efficiency could still be improved regarding the following points :

1.) simultaneous control of stepsize and order,

2.) computation of the *a priori* inclusion,

3.) choice of the local coordinate system (i.e. choice of the matrices A_j in the methods of Section 8),

4.) modifications in the case of stiff systems.

Kirlinger and Corliss [38] consider *implicit Taylor series methods* for *stiff problems* and partly apply them to interval methods. However, modifications for *stiff systems* are not useful unless the stepsize exceeds the stepsizes in explicit methods. Gong [26] has recently presented some ideas to verify *a priori* bounds for relatively large steps in stiff problems with certain stability properties.

Lohner also applies his method to *boundary value problems* using single or multiple shooting (see [47]). Other approaches in verifying and enclosing solutions of boundary value problems are possible. Some papers on this topic are presented in [88] and [89], for example.

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