# Taylor forms – use and limits

**Arnold Neumaier**

*Institut für Mathematik, Universität Wien*
*Strudlhofgasse 4, A-1090 Wien, Austria*
*email: Arnold.Neumaier@univie.ac.at*
*WWW: http://www.mat.univie.ac.at/~neum/*

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**Abstract.** This review is a response to recent discussions on the reliable computing mailing list, and to continuing uncertainties about the properties and merits of Taylor forms, multivariate higher degree generalizations of centered forms. They were invented around 1980 by Lanford, documented in detail in 1984 by Eckmann, Koch and Wittwer, and independently studied and popularized since 1996 by Berz, Makino and Hoefkens. A highlight is their application to the verified integration of asteroid dynamics in the solar system in 2001.

Apart from summarizing what Taylor forms are and do, this review puts them into the perspective of more traditional methods, in particular centered forms, discusses the major applications, and analyzes some of their elementary properties. Particular emphasis is given to overestimation properties and the wrapping effect. A deliberate attempt has been made to offer value statements with appropriate justifications; but all opinions given are my own and might be controversial.

**Keywords**: affine arithmetic, approximation order, asteroid dynamics, cancellation, centered form, cluster effect, computer-assisted proof, constraint propagation, dependence, interval arithmetic, overestimation, overestimation factor, quadratic approximation property, range bounds, rigorous bounds, slopes, Taylor-Bernstein method, Taylor form, Taylor model, Taylor series with remainder, ultra-arithmetic, verified enclosure, wrapping effect

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# Part 1: Properties and history of Taylor forms

## 1 Introduction

Taylor forms are higher degree generalizations of centered forms. They compute recursively a high order polynomial approximation to a multivariate Taylor expansion, with a remainder term that rigorously bounds the approximation error. Storage is proportional to $\binom{n+d}{d} = \binom{n+d}{n} = O(\max(n,d)^{\min(n,d)})$ for an approximation of degree $d$ in $n$ variables. The work is proportional to this number and to the number of arithmetic operations. Both counts may be much less for sparse problems, or when it is known that the function has low degree in some variables.

Rigorous multivariate Taylor arithmetic with remainder, for the four elementary operations and composition exists at least since 1984 (Eckmann et al. [30, 31]). Independently, a slightly different version of Taylor arithmetic with remainder has been made popular since 1996 under the name Taylor models by Martin Berz and his group; their papers [5, 6, 7, 8, 9, 43, 44, 45, 46, 90, 92] on Taylor models and their applications can be found at

`http://bt.pa.msu.edu/pub/papers/.`

An efficient implementation is freely available within the framework of the COSY INFINITY package (designed for beam physics applications) of Martin Berz at

`http://cosy.pa.msu.edu/.`

In the Eckmann et al. implementation, the polynomial coefficients are narrow intervals taking care of all rounding errors, and the remainder term is a simple norm bound. In the COSY implementation, the polynomial coefficients are floating point numbers and the remainder term is an interval; rounding errors are handled by a Wilkinson-style aposteriori correction technique. Some demonstrations in MAPLE (with a toy implementation for the univariate and bivariate case, without rounding error control) can be found in Corliss [21].

So far I have not seen any convincing evidence that the use of floating point numbers as coefficients is an essential improvement over using narrow interval coefficients. For many problems with significant input width, rounding errors only affect trailing digits and hence are completely immaterial. For problems where the input is close to the roundoff level, either a theoretical analysis, or a thorough comparison with an alternative implementation is needed to decide which approach is better. Unfortunately, the package of Eckmann is not available.

The various forms of Taylor arithmetic constitute a significant enhancement of the toolkit of interval analysis techniques. Indeed, interval coefficient forms were used by mathematical physicists to prove estimates important for computer-assisted proofs, and floating-point coefficient forms were used by Berz and his group to verify solutions of celestial mechanics problems that so far defied interval techniques. Berz and his group also used Taylor models for applications to multivariate integration over a box, differential algebraic equations and verified Lyapunov functions for dynamical systems.

The paper is organized as follows. In Part 1, we give a history of Taylor forms and their applications, with references to related work, in particular to centered forms, which are the

degree 1 case of Taylor forms. Known properties of Taylor forms are also reviewed, mainly in an essay style. We begin with the univariate case (Section 2), then look at the multivariate case (Section 3), give a precise review of approximation order (Section 4), and look in particular at range bounding in Taylor models (Section 5). Finally, we review applications to the verified integration of functions and initial-value problems (Section 6).

Part 2 gives a detailed mathematical analysis of centered forms, which applies also to Taylor forms in general. In Section 7, we introduce a distinction between different forms of overestimation, due to wrapping, cancellation, or dependence; then we discuss computable overestimation bounds in centered forms (Section 8) and a constraint propagation technique for improving bounds on centered forms (Section 9).

Part 3 gives a detailed mathematical analysis of some aspects of the particular class of Taylor forms referred to by Martin Berz as Taylor models, building (as far as available) upon published information about details of their implementation. We first look at rounding issues (Section 10), then at overestimation in Taylor models (Section 11), then at cancellation effects, the most used property of Taylor models (Section 12), investigate some wrapping properties of Taylor models first in discrete dynamical systems (Section 13), then in the enclosure of initial-value problems (Section 14).

Finally, some of the major findings are summarized in the conclusions (Section 15), and a long list of references invites the reader to deeper study.

**Notation.** In the following, the notation is as in my book [107]. In particular, intervals and boxes (= interval vectors) are in bold face, $\check{\mathbf{x}} = \operatorname{mid}\mathbf{x} = \frac{1}{2}(\overline{x} + \underline{x})$ denotes the midpoint and $\operatorname{rad}\mathbf{x} = \frac{1}{2}(\overline{x} - \underline{x})$ the radius of a box $\mathbf{x} \in \mathbb{IR}^n$, and inequalities are interpreted componentwise.

# 2 The univariate case

One-dimensional Taylor forms have a long history. In 1962, Moore [97, 98], in his groundbreaking Ph.D. thesis and book, (and many after him) used Taylor expansions with error intervals, but bounded the error terms using a separate calculation of an interval Taylor polynomial, which frequently gives unduly pessimistic bounds, especially if the original function has significant cancellation. Computing the bounds concurrently with the polynomial, as done by Eckmann and Berz, yields significantly sharper results; for Taylor forms of order 1, this is observed on p. 57 of my book [104]. Asymptotically, for sufficiently narrow intervals, one probably gains a factor of $d + 1$ for a method of order $d$; for the case $d = 1$, this follows easily from Proposition 2.12 of my book [104].

One-dimensional Taylor expansions with error intervals, and improved variants based on Tchebyshev and Bernstein expansions and residual enclosures were extensively used around 1980 by Krückeberg, Kaucher, Miranker and others, some of it under the name of ultra-arithmetic (or functoid), with a philosophy very close to that of Berz's approach; see, e.g., the book Kaucher & Miranker [58] and the papers [11, 36, 54, 59, 60, 61, 95, 96]. Applications to various functional equations are given in Dobner [28], Kaucher & Baumhof [56], Klein [67], Kaucher & Krämer [57].

The residual approach is based upon the observation that if $p(t)$ is a high order approximation to $y(t)$ then $y(t) = p(t) + e(t)$ with an error function $e(t)$ that consists of roundoff and a high order term; enclosing $e(t)$, given implicitly by a functional equation, therefore only needs intervals of tiny width at rondoff level (except at the highest order), which reduces the overestimation.

The technique did not catch on – since much of it was phrased in unnecessarily abstract terms that few were prepared to wade through; since the time was not yet ripe for doing extensive semisymbolic computations; and apparently also since the proponents did not continue their work. It would be time to reassess their methods and to put the valuable part into a more readable formal context.

The first (computer-assisted) proof of the Feigenbaum conjecture by Lanford [79] was based on complex Taylor arithmetic; a more developed form is in Eckmann & Wittwer [32]. Variants of such an arithmetic have been used for proving important estimates in quantum physics; see the review in Fefferman & Seco [37]. For related work on computer-assisted proofs in analysis see, e.g., [13, 14, 15, 29, 30, 68, 70, 71, 72, 80, 115, 121, 122] and several papers in [93].

A comparison of univariate Taylor forms and Tchebyshev forms in Kaucher & Miranker [60, p. 420f] suggests that expansions in Tchebyshev polynomials may be orders of accuracy more accurate than expansions in Taylor series. This is probably the case because high powers in multiplications are in Taylor forms simply replaced by their range, while in Tchebyshev forms they are replaced by their Tchebyshev approximations, which results in a much smaller remainder term.

# 3 The multivariate case

In more than one dimensions, first order Taylor forms are cheap; prominent examples are the slope-based centered form (Krawczyk & Neumaier [74], with improvements in Neumaier [104, pp. 61–64], Rump [119] and Kolev [73]) with slopes computed by automatic differentiation, implemented, e.g., in the INTLAB package by Rump [120].

First order Taylor models are a simplified version of these in which the width of the linear coefficients is moved to the remainder term. They were used, for example, in Theorem 2.2 of my paper [103], and the quadratic approximation order of the resulting linear enclosures of the implicit functions is proved.

Comparisons between first order Taylor models and the mean value form, or the more efficient centered forms based on slopes are not available. It seems that what is more advantageous depends on details on estimating the remainder terms. Because of the subdistributive law, slopes are more accurate than simple implementations of Taylor forms, but if squares are given a special treatment, Taylor forms have an asymptotic advantage in the second order part of the width of a factor of $1/2$ in one dimension and (for a general quadratic contribution with coefficients of the same order) of $1 - \frac{1}{2n}$ in dimension $n$.

Other first order Taylor forms of potential interest were introduced by de Figueiredo &

Stolfi [26] under the name of affine arithmetic; see also [20, 25, 2, 27]. Their distinguishing property is that the function is expanded not only in the initial parameters but also in intermediate intervals resulting from the nonlinearities. Thus affine arithmetic seems to be something intermediate between Taylor forms and zonotopes (Kühn [77]), and perhaps has some wrapping reducing properties. However, numerical comparisons are available only against naive interval evaluations, not against centered forms based on slopes, so that an evaluation of their merits is currently not possible.

Details on higher order multivariate Taylor forms appear first 1984 in 2 complex dimensions in Eckmann, Koch & Wittwer [30] (with the remark on p. 48, 'we leave to the reader the details of extension to more variables or the reduction to one variable'). They give full implementation details (and Fortran code) on rounding, arithmetic operations, implicit functions (which gives division and roots, as explained in Eckmann et al. [31, p. 154]), and the composition of functions (which gives arbitrary analytic standard functions for which polynomial enclosures with error bounds are available).

A recursive PASCAL-SC implementation of real multivariate Taylor forms (from 1987) in arbitrary dimensions is described in Kaucher [55], and applied to the solution of hyperbolic partial differential equations.

A different, more efficient C++ library (from 1996, calling Fortran programs translated into C) of multivariate Taylor forms in arbitrary dimensions, called Taylor models, and freely available for academic research, is described in Makino & Berz [91, 90]; the rounding error control used was described in a lecture given at the SIAM Workshop on Validated Computing 2002 [123].

Koch [68, Section 6] describes a (public domain) ADA95 implementation [69] of a 3-dimensional function arithmetic for functions in $(x, y, z)$ which are $2\pi$-periodic in $x$ and $y$, and either even or odd under $(x, y) \to (-x, -y)$. Earlier, a function arithmetic for univariate periodic functions was given by Kaucher & Baumhof [56].

For reasonably narrow boxes, higher order Taylor forms (which are substantially more expensive) compute a polynomial with a tiny error interval, if the domain of analyticity of the function is large. The advantage over traditional centered forms is that, using a fixed basis of polynomials for the approximation, one can cancel a significant amount of dependence by summing the corresponding contributions into a single real coefficient, and the remaining dependence is shifted to the high order remainder term, which under the stated conditions is tiny even if much overestimation occurs in its computation. (In the case of preconditioning nonlinear systems, this reduction of overestimation was observed independently by Hansen [41], although he did not develop his observation into a general algorithm.)

The Taylor approach encloses function values at point arguments to high order, and hence the graph of the function. This makes the method highly accurate for some applications like integration over a box. But applications that need a good enclosure of the range of the function are different since in this case interval evaluations of the Taylor form are needed, and these are nontrivial. Simple interval evaluation of all Taylor forms (in power or Horner form) for narrow intervals only has a quadratic approximation order, and suffers from the same problem as other centered forms near stationary points.

Over sufficiently wide boxes, the Taylor form shares the fate of any centered form, that it

usually gives a large overestimation and may even be poorer than naive interval evaluation. It is not designed for such applications, and global optimization methods should be used instead. (Possibly, global optimization methods may benefit from using Taylor forms as part of their bag of tricks.) The domain of interest is that of complicated functions whose variables range over intervals of engineering accuracy (inaccuracy inherent in data obtained by measurements, up to a few percent relative error, and in certain cases more).

# 4 Approximation order

While it is difficult to give any meaningful general analysis for the quality of a range enclosure over wide intervals, asymptotic results for narrow intervals are possible and have important applications in global optimization and global zero finding.

A method that produces for every arithmetic expression $f(x)$ in $n$ variables $x_1, \ldots, x_n$ and every box $\mathbf{x}$ contained in some fixed box $\mathbf{x}^{\text{ref}}$ an interval $f_{\text{enc}}(\mathbf{x})$ is said to enclose (in $\mathbf{x}^{\text{ref}}$) the range with **approximation order** $s$ if, for all $\varepsilon \in \ ]0,1]$ and every box $\mathbf{x} \subseteq \mathbf{x}^{\text{ref}}$ of maximal width $\varepsilon$,

$$f(x) \in f_{\text{enc}}(\mathbf{x}) \quad \text{for all } x \in \mathbf{x} \tag{1}$$

and the width of $f_{\text{enc}}(\mathbf{x})$ differs from that of the range $\{f(x) \mid x \in x\}$ by not more than $C\varepsilon^s$ with some constant $C$ depending on the function and the reference box $\mathbf{x}^{\text{ref}}$ but not on $\mathbf{x}$ or $\varepsilon$. The method has approximation order $s$ without reference to a function or a box, if it has this approximation order for (at least) all polynomials and all boxes. (This is a minimal consensus, consistent with the recent literature; cf. Neumaier [104, Chapter 2], Kearfott [63, Definition 1.4], Jaulin et al. [53, p. 35].) The approximation order is **linear** if $s \geq 1$, **quadratic** if $s \geq 2$, and **cubic** if $s \geq 3$.

In view of recent misunderstandings, it is important to note that order statements are not restricted to boxes with a fixed midpoint. Indeed, the independence of the location of the midpoint is essential in applications, since the frequently needed subdivision process could not work if the midpoint is to be kept fixed.

Under mild conditions excluding near-singular cases such as $\sqrt{[h,3h]}$, interval evaluation has linear approximation order, and centered forms have the quadratic approximation order, see, e.g., Chapter 2.3 of my book [104]. Thus, for boxes sufficiently far away from stationary points, the overestimation factor

$$p := (\text{width of computed range}/\text{width of true range} - 1) * 100\% \tag{2}$$

is proportional to the width of the input box, indicating satisfactory enclosures. Upper bounds on $p$ can be computed from the information in a centered form at hardly any additional cost, see Section 8 below. Thus one knows whether one was good enough.

A bicentered form Neumaier [104, p. 59] frequently produces the exact range of the polynomial, namely if the box is narrow enough and sufficiently far away from a stationary point. However, the method is only of second order because the defining property fails for boxes sufficiently close to or containing a stationary point.

But near stationary points of the function, where the true range is of second order, typically poor overestimation factors result for arbitrarily narrow intervals. As observed by Kearfott & Du [65], this causes severe slowdown in branch and bound methods. Indeed, branch and bound methods for minimizing a function in a box (or a more complex region) frequently have the difficulty that subboxes containing no solution cannot be easily eliminated if there is a nearby good local minimum. This has the effect that near each zero, many small boxes are created by repeated splitting, whose processing may dominate the total work spent on the global search.

This so-called cluster effect was explained and analyzed by Kearfott & Du [65]. They showed that it is a necessary consequence of range enclosures with less than cubic approximation order, which leave an exponential number of boxes near a minimizer uneliminated. If the order is $< 2$, the number of boxes grows exponentially with an exponent that increases as the box size decreases; if the order is 2, the number of boxes is roughly independent of the box size but is exponential in the dimension. For sufficiently ill-conditioned minimizers, the cluster effect occurs even with methods of cubic approximation order. (There are other methods, e.g., verifying Fritz John conditions that can be used to fight the effect, except in the ill-conditioned case. See the book by Kearfott [63].)

The cluster effect happens near all local minimizers with a function value close to or below the best function value found. So if there is a unique global minimizer, if all other local minima have much higher function values, and a point close to the global minimizer is already known then the cluster effect only happens near the global minimum. But the neighborhood in which it happens may be quite large, and while the global optimum has not yet been located it will appear also at other minimizers.

For finding all zeros of systems of equations by branch and bound methods, there is also a cluster effect. An analogous analysis by Neumaier & Schichl [109] shows that one order less is sufficient for comparable results. Thus first order methods (interval evaluation and simple constraint propagation) lead to an exponential cluster effect, but already second order methods based on centered forms eliminate it, at least near well-conditioned zeros. For singular zeros, the cluster effect persists with second order methods; for ill-conditioned zeros, the behavior is almost like that for singular zeros since the neighborhood where the asymptotic result applies becomes tiny.

Higher than second order methods were first considered in the univariate case by Cornelius & Lohner [23], where they are cheap and work quite well. A refinement of their methods is presented in Neumaier [104, Chapter 2.4].

# 5 Range bounding in Taylor models

For range bounding, the Taylor approach only reduces the problem of bounding the range of a factorable function to that of bounding the range of a polynomial in a small box centered around 0, and the Taylor form is as good or bad as the way used to solve the latter problem.

At the end of the paper [23] it is mentioned that higher than second order multivariate enclosures are difficult because of the difficulty of getting high order enclosures for polynomials.

An extensive comparison of range enclosure methods on polynomials in 1 and 8 variables is given in the thesis by STAHL [124].

KEARFOTT & ARAZYAN [64] give some initial results indicating that sometimes Taylor models (apparently with simple Horner evaluation of the polynomial part) help in a global optimization context, but they only seem to delay the curse of dimensionality (i.e., the exponential growth of work with dimension on many problem classes) very little, in contrast to claims in HOEFKENS et al. [44, Section 2.2] that Taylor models 'offer a cure for the dimensionality curse'.

If the nonlinear terms contribute less than the linear terms (such as in normal form applications, or when boxes are narrow), the interval evaluation of the approximation polynomial is good enough (quadratic approximation property), and outperforms methods based on simple slopes if the original function incurs much dependence. Using a bicentered form to evaluate the approximation polynomial may even result in the exact range of the polynomial; in this case, the resulting range of the original function has a high order accuracy, with overestimation of order (polynomial degree +1).

If terms of all orders contribute strongly, the input box must be considered as large for this problem, since the asymptotic behavior is no longer visible, and accuracy will be poor (and perhaps poorer than centered forms using slopes only).

If high order terms are small but the second order terms dominate (which often happens when the intervals get a little wider), the interval evaluation of the approximation polynomial (both in power form and in Horner form) still suffers from dependence (though in a more limited way), and better methods are needed to get good bounds on the range. A natural goal is to have a method overestimating the width by at most a fixed small percentage defined by the user, e.g., $p <= 5\%$.

The thesis MAKINO [90] contains on pp.128–130 a rough outline of a *linear dominated range bounder* for $x \in [z-r, z+r]^d$. (A generalized version of this recipe is derived in detail in Section 9.) Let $c^T x$ be the linear part of a Taylor model, and let $d$ be the width of an enclosure for the range of the higher order part (including remainder). Then to compute a better upper bound on the Taylor polynomial, the lower bound for $x_j$ can be increased to $\max(z-r, z+r-d/|c_j|)$, since the maximizer can be at most $d/c_j$ away from the maximizer of the linear part. Now recenter the polynomial part of the Taylor model in the new box by a complete Horner scheme (one has take care of roundoff, but no details are given) and iterate this until the box size stabilizes. In regions where the function is monotonic, this frequently gives a much better upper bound. An analogous process frequently improves the lower bound.

But for $n > 2$ and the function

$$f(x) = -x_1^2 - \ldots - x_n^2 \quad \text{in any box } \mathbf{x} = [0.1h, 1.1h]^n \tag{3}$$

of width $h > 0$, the linear dominated range bounder stalls immediately and therefore gives a range overestimating the true range by $O(h^2)$.

This proves that for $n > 2$, Taylor forms (at least in their current implementation) do not have cubic approximation order. (It also shows that successes in dimension $\leq 2$ can be very

misleading about the performance in general.) That cubic approximation order is unlikely to be achieved with simple methods (Taylor based or not) is also a consequence of results by KREINOVICH [76], which show that range estimation over a box of maximal width $\varepsilon$ with accuracy $O(\varepsilon^2)$ (a simple consequence of cubic approximation order) is NP-hard. (Another negative result for higher than second order is in HERTLING [42], but the paper makes very strong assumptions that are easily avoided in practice.)

Another suggestion in Makino's thesis [90, pp.123–127] is to evaluate the exact range of quadratics and to treat higher order terms by simple interval arithmetic. By CORNELIUS & LOHNER [23, Theorem 4], this way of proceeding ensures the cubic approximation property.

In [90], the exact range of the quadratic part is computed recursively, using $2^{n-3}n!$ case distinctions. This is an inefficient version of a process called peeling, discussed in greater generality in KEARFOTT [63, Section 5.2.3] (but originating in KEARFOTT [62]). For quadratics, it amounts to solving at most $3^n$ linear systems to find all those Kuhn-Tucker-points of the quadratic form on the box with a function value below (for the minimum; above for the maximum) that of the best point found. The work is worst case exponential, but in Kearfott's version possibly much faster on the average case. Tests on random problems with suitable statistics would be interesting.

The Taylor-Bernstein method of NATARAJ & KOTECHA [99, 100] is also only worst case exponential but possibly much faster on the average case. Moreover, it produces highly accurate enclosures for the range also for polynomials of higher degree, and therefore (if applied to the polynomial part of a Taylor form) gives an approximation order one higher than the degree of the Taylor polynomial. On the other hand, the work per split is proportional to $\binom{n+d}{d} = \binom{n+d}{n} = O(\max(n,d)^{\min(n,d)})$, so that the method is limited to small values of min(degree,dimension).

To get a feeling for the dependence of a range bounding method on the dimension, a simple test problem with some dependence (each variable occurs $n$ times) is

$$f(x) = \sum_{i=1}^{n}(x_i - (n+1)^{-2})^2 - \sum_{i=2}^{n} x_i x_{i-1}$$

on the box with n components $[-0.25, 0.25]$. The exact range is

$$\Big[ -\frac{n(n+4)(n-1)}{6(n+1)^4}, \frac{2n-1}{16} + \frac{1-(-1)^n}{4(n+1)^2} + \frac{n}{(n+1)^4} \Big];$$

the lower bound is attained at the point with $x_i = \frac{i}{n+1}(1-\frac{i}{n+1})$ for all $i$, and the upper bound at the point with $x_i = 0.25(-1)^i$ for all $i$. Since the problem is quadratic, peeling produces the exact range, too. It would be interesting to see how peeling and the Taylor-Bernstein method compare in speed, and at which dimension the methods start to become impractical.

# 6 Applications to verified integration

Here I concentrate on applications to verified integration (of functions, ordinary differential equations, and differential-algebraic equations) reported by Berz, Makino and Hoefkens with the COSY implementation of their Taylor models.

Berz & Makino [7] apply Taylor models to multivariate integration over a box in dimensions 1,3,4,6, and 8. Their paper begins with "The verified solution of one- and higher-dimensional integrals is one of the important problems using interval methods in numerics", and quotes Kaucher & Miranker [58] (who treat univariate integration and ultra arithmetic, potentially useful for higher dimensions, too) and three books which have nothing to do with integration of functions. Not mentioned is other past work on verified integration (in up to 3 dimensions); see Storck [126, 127, 128], Holzmann et al. [47], Lang [81, 82], Chen [18], Wedner [131]). For integration in one dimension, there are highly efficient algorithms by Petras [110] related to older work by Eiermann [33, 34], and promising theory (Petras [111]) for higher dimensions. No comparison between the methods exists. Only for verified quadrature in high dimensions, the Taylor approach seems to have currently no real competition.

In applications to ODE's, Taylor models are claimed to lead to a "practical elimination of the wrapping effect", see Berz [5]. Such a claim is unfounded, being based on no theory and very few examples only. Taylor models in themselves are as prone to wrapping as other naive approaches such as simple integration with a centered form, since wrapping in the error term cannot be avoided. For a $d$th order method, the error term is of order $O(\delta^{d+1}) + O(\varepsilon)$ for a box of width of order $\delta$ and calculations with machine accuracy $\varepsilon$; and the rounding errors suffice for most problems to quickly blow up the results to a meaningless width.

But for highly nonlinear systems and higher orders, the wrapping is less severe than for naive integration, due to the ability of Taylor models to represent uncertainty sets with curved boundary. To keep the wrapping effect at a tolerable level, special measures must be taken, similar to those discussed in the literature (Jackson [48], Lohner [83] , Kühn [77]); Berz does it in COSY with an additional technique called 'shrink wrapping', described in a lecture given at the SIAM Workshop on Validated Computing 2002 [123]. It can be considered as a slightly modified nonlinear version of the parallelepiped method, or a nonlinear version of a simplified zonotope technique, cf. Kühn [77].

Performance of shrink wrapping is likely to depend on spectral properties of the system considered. Nedialkov & Jackson [101] gave an excellent theoretical analysis of traditional enclosure methods for linear constant coefficient problems; their discussion of the parallelepiped method (to which shrink wrapping seems to reduce in this particular case) suggests that, unlike the QR technique of Lohner [83, 85, 86, 87, 88] implemented in the AWA program [84], shrink wrapping is not flexible enough to handle well the case when along part of the trajectory the Jacobian has eigenvalues of significantly different real part, except for highly dissipative systems (such as the Lorentz equation), where the wrapping is compensated by drastic volume reductions in phase space. In particular, unless coupled with other wrapping-reducing techniques, shrink wrapping is unlikely to work well on volume preserving systems with local instabilities.

However, Taylor models with shrink wrapping are reported to work *exceedingly well* for volume-preserving dynamical systems that are everywhere locally stable, i.e., where all eigenvalues of all Jacobians in a neighborhood of the trajectory are purely imaginary; this happens, e.g., for stable Hamiltonian systems. (The defect-based method in Kühn [78] also seems to have this property. In both cases, I have no proof for my impression, so these statements should rather be considered as conjectures, for which proofs would certainly be of very high interest.)

For example, with step size control and suitably chosen order (there seems to be no order control), COSY very much outperforms Lohner's AWA on celestial mechanics problems, according to pp. 154–158 of the dissertation by Hoefkens [43]. AWA is able to verify only a year of a much simpler six-dimensional Kepler problem (on which the Taylor model implementation in COSY was over 1000 times slower but four orders of magnitude more accurate) while Taylor models handled successfully the integration of a complicated model over 10 years, with only moderate wrapping effect. This is apparently due to the use of shrink wrapping together with the ability of Taylor models to represent uncertainty sets with curved boundary, while AWA has to use parallelepipeds and is therefore much less adaptive.

(Kyoko Makino optimized both the input (right hand side and parameters) of AWA and COSY-VI, her current version of the Taylor model package, by careful choices of the control parameters and the form of the expressions, and found that the overestimation per revolution of the asteroid in the case of COSY-VI was about 1000 times less than that of AWA, but took about 60 times more CPU time. In the optimized version, AWA was able to complete about three revolutions only, at which time the COSY enclosures were still below drawing resolution.)

Celestial mechanics poses many other interesting challenges for verified computations; see, e.g., Celletti & Chierchia [14, 15, 16, 17], who treat among others the system Sun – Jupiter – Ceres, but are able to do the verification only for unrealistic mass ratios.

A nice and deep mathematical analysis of an algorithm similar to Lohner's has been carried out in the book by Eijgenraam [35]. In particular, there was a proof that (assuming exact arithmetic, and under natural conditions related to the global existence of trajectories) one can rigorously enclose an ensemble of trajectories over arbitrarily long times if the initial width of the ensemble is sufficiently small (depending on the time span). It would be interesting to extend this in my opinion very important work to Taylor forms, and to the case including rounding errors.

Lohner's AWA method is able to propagate the dependence on initial conditions throughout the integration, while shrink wrapping loses this dependence upon its first use. Thus, unlike AWA, shrink wrapping is (in its present form) not applicable to verifying the solution of boundary-value problems by means of multiple shooting. For work related to AWA see also Kerbl [66], Rihm [117], Gong [40], Corliss & Rihm [22], Stauning [124], Nedialkov et al. [102] and Janssen [51].

Berz and his group also used Taylor models for applications to differential algebraic equations (Hoefkens et al. [44, 45], following earlier work by Pryce [113, 114]), and to verified Lyapunov functions (Berz & Makino [8]) for dynamical systems.

# Part 2: Analysis of centered forms

Taylor forms, at least if evaluated in a Horner-like manner, can be viewed as generalized centered forms in which (for the Taylor model variant) the constant term is expanded by the remainder term to give a thick interval constant. Some of the properties of Taylor forms can

therefore be analyzed in terms of general centered forms which are essentially Taylor forms of degree 1.

# 7 Overestimation

It is well-known that interval calculations generally overestimate the range of an expression, except under special circumstances. In the following, we distinguish three sources of overestimation:

**Wrapping** relates to overestimation due to the depth of the computational graph, caused by long sequences of *nested* operations depending on a limited number of variables only, which also magnifies bounds on rounding errors and hence can give wide meaningless results even for problems with exact data. **Cancellation** relates to overestimation due to expressions containing at least one addition or subtraction where, in floating point arithmetic, the result has much smaller magnitude than the arguments; in interval arithmetic, the width is additive instead of cancelling, leading to large overestimation in such cases. **Dependence** refers to multiple occurrences of one or several variables, even in the absence of cancellation or deeply nested computations. Thus both wrapping and cancellation are special forms of dependence.

This definition of wrapping (conforming in spirit with the looser definition given in Lohner [89]) is slightly more general than the traditional view, which restricts the notion of wrapping to nested operations in form of a discrete dynamical system

$$y_{t+1} = F_t(y_t) \tag{4}$$

with $y_t$ of fixed dimension, but it is equivalent to this if one removes the fixed dimension constraint. Wrapping of the form (4) is one of the most frequent ways wrapping occurs. However, in the generalized view of wrapping, other phenomena such as the blow up of interval Gauss elimination are covered, too. Indeed, a linear discrete dynamical system can be viewed as a triangular system of linear equations, and then the wrapping of the dynamical system shows as blow up in Gauss elimination (Neumaier [105]). Further important examples of wrapping in other contexts (difference equations, automatic differentiation) are given in Lohner [89].

The amount of wrapping is related to the level of nestedness, i.e., the depth of the reduced computational tree obtained by combining linear combinations into single nodes. However, the size and sign of the coefficients involved determines how much wrapping actually occurs, and a complete analysis is possible only for well-structured simple cases.

Wrapping is primarily a phenomenon of discrete dynamical systems and other recurrent computations. However, it also arises in the verification of solutions of ordinary differential equations, because usually a long trajectory must be split into short pieces that can be verified. (Possible exceptions to this are the techniques of Kühn [78] and Neumaier [106], which give conditions under which solutions can be verified over long time in a single verification step.) The associated discrete dynamical system is therefore that propagating the solution from one node of the time discretization to the next node. Therefore, solving the wrapping problem for ordinary differential equations is essentially equivalent to solving the wrapping problem in the discrete case.

# 8 Overestimation in centered forms

For sufficiently narrow intervals, overestimation due to arbitrary dependence can be drastically reduced by means of centered forms, and, except near stationary points, virtually eliminated. This is due to the quadratic approximation property of centered forms. However, since the latter is an asymptotic property only, it sometimes (in cases with significant wrapping or cancellation) holds only for quite narrow boxes.

Therefore it is useful to have computable quantities that show to which extent the reduction is effective in each particular case. In this section we derive overestimation bounds for centered forms that allow the explicit computation of an upper bound to the overestimation factor (2). They generalize the bounds from KRAWCZYK & NEUMAIER [75], [104, Theorem 2.3.3] (which has a correct statement but an erroneous proof) and [103, Theorem 4.1] to the case of thick constant terms as they occur in Taylor models. But this generalization is also of interest for ordinary centered forms, where rounding errors lead to narrow intervals for the constant term. (The bounds in [75, 104, 103] are valid only in exact arithmetic, but see RUMP [118] for rigorous rounding error control.)

The **Hausdorff distance** of two intervals $\mathbf{a}, \mathbf{b} \in \mathbb{IR}$ is the number

$$q(\mathbf{a}, \mathbf{b}) := \max(|\underline{a} - \underline{b}|, |\overline{a} - \overline{b}|),$$

the **mignitude** $\langle \mathbf{a} \rangle$ and the **zerolength** $\operatorname{zl} \mathbf{a}$ of $\mathbf{a} \in \mathbb{IR}$ are

$$\langle \mathbf{a} \rangle := \min\{|a| \mid a \in \mathbf{a}\} = \begin{cases} 0 & \text{if } 0 \in \mathbf{a}, \\ \min(|\overline{a}|, |\underline{a}|) & \text{if } 0 \notin \mathbf{a}, \end{cases},$$

$$\operatorname{zl} \mathbf{a} := \operatorname{width}\{|a| \mid a \in \mathbf{a}\} = \begin{cases} |\mathbf{a}| & \text{if } 0 \in \mathbf{a}, \\ |\overline{a} - \underline{a}| & \text{if } 0 \notin \mathbf{a}. \end{cases}$$

For $\mathbf{x} \in \mathbb{IR}^n$ and $\mathbf{A} \in \mathbb{IR}^{m \times n}$, we define $\langle \mathbf{x} \rangle \in \mathbb{R}^n$ and $\operatorname{zl} \mathbf{A} \in \mathbb{R}^{m \times n}$ by

$$\langle \mathbf{x} \rangle_i = \langle \mathbf{x}_i \rangle, \quad (\operatorname{zl} \mathbf{A})_{ik} = \operatorname{zl} \mathbf{A}_{ik}. \tag{5}$$

From NEUMAIER [103, Lemma 1.1.(ii)], we have for $\mathbf{a}, \mathbf{b} \in \mathbb{IR}^n$,

$$\operatorname{rad}(\mathbf{a}^T \mathbf{b}) \le (\langle \mathbf{a} \rangle + 2 \operatorname{rad} \mathbf{a})^T \operatorname{rad} \mathbf{b} \quad \text{if } 0 \in \mathbf{b}. \tag{6}$$

**8.1 Theorem.** *Let $F : \mathbf{x} \subseteq \mathbb{R}^n \to \mathbb{R}^m$ be a function, $z \in \mathbf{x}$ and*

$$F(x) \in \mathbf{a} + \mathbf{A}(x - z) \quad \textit{for all } x \in \mathbf{x}. \tag{7}$$

*Then*

$$\mathbf{w} := \{F(x) \mid x \in \mathbf{x}\} \subseteq \mathbf{a} + \mathbf{A}(\mathbf{x} - z) =: \mathbf{w}', \tag{8}$$

*and*

$$q(\mathbf{w}, \mathbf{w}') \le 2 \operatorname{rad} \mathbf{a} + (\operatorname{zl} \mathbf{A})|\mathbf{x} - z| \tag{9}$$

$$0 \le \operatorname{rad} \mathbf{w}' - \operatorname{rad} \mathbf{w} \le 2 \operatorname{rad} \mathbf{a} + 2(\operatorname{rad} \mathbf{A}) \operatorname{rad} \mathbf{x}. \tag{10}$$

*Proof.* If $m > 1$, we get the assertions from that for $m = 1$ by applying it to each component of $F(x)$ separately. Therefore it suffices to prove the assertions in the case where $F(x)$ is real-valued ($m = 1$). Then $\mathbf{a}$ is an interval and $\mathbf{A} = \mathbf{b}^T$ is a row vector. Define the vector $x' \in \mathbb{R}^n$ with components

$$\begin{aligned} x'_k &= \underline{x}_k \quad \text{if } k \in K^+ = \{k \mid \underline{b}_k > 0\}, \\ x'_k &= \overline{x}_k \quad \text{if } k \in K^- = \{k \mid \overline{b}_k < 0\}, \\ x'_k &= z_k \quad \text{if } k \in K^0 = \{k \mid 0 \in \mathbf{b}_k\}. \end{aligned}$$

Then

$$F(x') \in \mathbf{a} + \mathbf{b}^T(x' - z) = \mathbf{a} + \sum_k \mathbf{b}_k(x'_k - z_k),$$

$$\underline{w} \le F(x') \le \overline{a} + \sum_{k\in K^+} \underline{b}_k(\underline{x}_k - z_k) + \sum_{k\in K^-} \overline{b}_k(\overline{x}_k - z_k), \tag{11}$$

$$\mathbf{w}' = \mathbf{a} + \mathbf{b}^T(\mathbf{x} - z) = \mathbf{a} + \sum_k \mathbf{b}_k(\mathbf{x}_k - z_k), \tag{12}$$

$$\underline{w}' \ge \underline{a} + \sum_{k\in K^+} \overline{b}_k(\underline{x}_k - z_k) + \sum_{k\in K^-} \underline{b}_k(\overline{x}_k - z_k) - \sum_{k\in K^0} |\mathbf{b}_k||\mathbf{x}_k - z_k|, \tag{13}$$

hence

$$\begin{aligned} \underline{w} - \underline{w}' &\le \overline{a} - \underline{a} - \sum_{k\in K^+} (\overline{b}_k - \underline{b}_k)(\underline{x}_k - z_k) + \sum_{k\in K^-} (\overline{b}_k - \underline{b}_k)(\overline{x}_k - z_k) + \sum_{k\in K^0} |\mathbf{b}_k||\mathbf{x}_k - z_k| \\ &\le 2\operatorname{rad}\mathbf{a} + \sum_{k\in K^+} \operatorname{zl}\mathbf{b}_k|\mathbf{x}_k - z_k| + \sum_{k\in K^-} \operatorname{zl}\mathbf{b}_k|\mathbf{x}_k - z_k| + \sum_{k\in K^0} \operatorname{zl}\mathbf{b}_k|\mathbf{x}_k - z_k|, \end{aligned}$$

giving

$$\underline{w} - \underline{w}' \le 2\operatorname{rad}\mathbf{a} + (\operatorname{zl}\mathbf{b})^T|\mathbf{x} - z|. \tag{14}$$

Changing the sign of $F$, $\mathbf{a}$, and $\mathbf{b}$ changes the sign of $\mathbf{w}$ and $\mathbf{w}'$; applying (11) and (14) to this situation and noting that multiplication by $-1$ interchanges lower and upper bounds gives the relations

$$\overline{w} \ge \underline{a} + \sum_{k\in K^+} \underline{b}_k(\overline{x}_k - z_k) + \sum_{k\in K^-} \overline{b}_k(\underline{x}_k - z_k), \tag{15}$$

$$\overline{w}' - \overline{w} \le 2\operatorname{rad}\mathbf{a} + (\operatorname{zl}\mathbf{b})^T|\mathbf{x} - z|, \tag{16}$$

since $\operatorname{rad}(-\mathbf{a}) = \operatorname{rad}\mathbf{a}$ and $\operatorname{zl}(-\mathbf{b}) = \operatorname{zl}\mathbf{b}$. Since $\mathbf{w} \subseteq \mathbf{w}'$, the Hausdorff distance is

$$q(\mathbf{w}, \mathbf{w}') = \sup(\underline{w} - \underline{w}', \overline{w}' - \overline{w}),$$

and the assertion (9) follows from (14) and (16). Combining (11) and (15) gives

$$\begin{aligned} \operatorname{rad}\mathbf{w} &= \tfrac{1}{2}(\overline{w} - \underline{w}) \\ &\ge \frac{1}{2}\Big(\underline{a} - \overline{a} + \sum_{k\in K^+} \underline{b}_k(\overline{x}_k - \underline{x}_k) + \sum_{k\in K^-} \overline{b}_k(\underline{x}_k - \overline{x}_k)\Big) \\ &= -\operatorname{rad}\mathbf{a} + \textstyle\sum\langle\mathbf{b}_k\rangle \operatorname{rad}\mathbf{x}. \end{aligned}$$

Since by (12) and (6),

$$\operatorname{rad}\mathbf{w}' = \operatorname{rad}\mathbf{a} + \operatorname{rad}(\mathbf{b}^T(\mathbf{x} - z)) \le \operatorname{rad}\mathbf{a} + (\langle\mathbf{b}\rangle + 2\operatorname{rad}\mathbf{b})^T \operatorname{rad}(\mathbf{x} - z)$$

and $\operatorname{rad}(\mathbf{x} - z) = \operatorname{rad}\mathbf{x}$, (10) follows by taking differences. □

# 9 Improving bounds from centered forms

The location of the arguments where the extrema of a function in a box are attained can be obtained by global optimization techniques, which also yield a (within rounding accuracy) precise range. Apart from the branch-and-bound principle and the traditional interval techniques discussed in KEARFOTT [63], there are constraint propagation techniques (see, e.g., VAN HENTENRYCK et al. [129] or NEUMAIER et al. [108]) that use bounds on the objective function to tighten the region where a minimizer or maximizer may occur.

On sufficiently narrow boxes sufficiently far away from stationary points, the minimum and maximum is always attained on the boundary, and constraint propagation applied to the centered form [129, p. 126f] typically reduces the domain to a small slice in all components where the gradient is sufficiently far from zero.

Explicit formulas are given in the following result, which generalizes an observation of MAKINO [90, pp. 128-130] for bounding polynomials in a box symmetric about zero.

**9.1 Theorem.** *Let $f : \mathbf{x} \subseteq \mathbb{R}^n \to \mathbb{R}$ be a function, $z \in \mathbf{x}$, and let $\mathbf{a} \in \mathbb{IR}, \mathbf{b} \in \mathbb{IR}^n$ be such that*

$$f(x) \in \mathbf{a} + \mathbf{b}^T(x - z) \quad \text{for all } \ x \in \mathbf{x}. \tag{17}$$

*If $x', x'' \in \mathbf{x}$ are extremal points of $f$ in $\mathbf{x}$,*

$$f(x') \le f(x) \le f(x'') \quad \text{for all } \ x \in \mathbf{x}, \tag{18}$$

*then, for any $i$ with*

$$|\check{b}_i|(\overline{x}_i - \underline{x}_i) > \delta := \overline{a} - \underline{a} + (\overline{b} - \underline{b})^T|x - z|, \tag{19}$$

*we have*

$$x_i' \in \begin{cases} [\underline{x}_i, \underline{x}_i + \delta/|\check{b}_i|] & \text{if } \check{b}_i > 0, \\ [\overline{x}_i - \delta/|\check{b}_i|, \overline{x}_i] & \text{if } \check{b}_i < 0, \end{cases} \tag{20}$$

$$x_i'' \in \begin{cases} [\underline{x}_i, \underline{x}_i + \delta/|\check{b}_i|] & \text{if } \check{b}_i < 0, \\ [\overline{x}_i - \delta/|\check{b}_i|, \overline{x}_i] & \text{if } \check{b}_i > 0. \end{cases} \tag{21}$$

*(In finite precision arithmetic, directed upward rounding of $\delta$ and outward rounding of the new intervals are needed.)*

*Proof.* Define

$$\tilde{f}(x) := \check{a} + \check{b}^T(x - z).$$

Since $x - z$ is thin, we have for $x \in \mathbf{x}$,

$$f(x) - \tilde{f}(x) \in \mathbf{a} - \check{a} + (\mathbf{b} - \check{b})^T(x - z) \subseteq \frac{1}{2}[-\delta, \delta],$$

hence,

$$\begin{aligned} |f(x) - f(x') - \check{b}^T(x - x')| &= |(f(x) - \tilde{f}(x)) - (f(x') - \tilde{f}(x'))| \\ &\le |f(x) - \tilde{f}(x)| + |f(x') - \tilde{f}(x')| \le \tfrac{1}{2}\delta + \tfrac{1}{2}\delta. \end{aligned}$$

In view of (18), we conclude that

$$0 \le f(x) - f(x') \le \check{b}^T(x - x') + \delta \quad \text{for all } x \in \mathbf{x}.$$

Therefore,

$$0 \le \inf_{x \in \mathbf{x}} \check{b}^T(x - x') + \delta = \delta - \sum_{\check{b}_i > 0} |\check{b}_i|(x'_i - \underline{x}_i) - \sum_{\check{b}_i < 0} |\check{b}_i|(\overline{x}_i - x'_i).$$

For $i$ with $\check{b}_i > 0$, we conclude that $0 \le \delta - |\check{b}_i|(x'_i - \underline{x}_i)$, while for $i$ with $\check{b}_i < 0$, we conclude that $0 \le \delta - |\check{b}_i|(\overline{x}_i - x'_i)$. This implies (20). But (20) improves upon the trival bound $x'_i \in [\underline{x}_i, \overline{x}_i]$ only if (19) holds.

Finally, by applying the argument to $-f$ in place of $f$, we obtain (21). □

Thus, if (19) holds for at least one index $i$, the range bounding problem can be split into a minimization and a maximization problem over a reduced box, and by recalculating an enclosure of the form (17) (i.e., a centered form) on the reduced box, the process can be iterated, and usually yields quite tight bounds on the range.

In practice, (19) is satisfied for some $i$ if $\mathbf{x}$ is sufficiently narrow, and no stationary point of $f$ is in $\mathbf{x}$ or close to $\mathbf{x}$.

# Part 3: Analysis of Taylor models

Here we analyze more specific features of Taylor models. Apart from specific implementation issues, most of what is said remains more or less valid for arbitrary Taylor forms.

## 10 Taylor models and rounding

A **Taylor model** of order $d$ (Makino & Berz [91]) is a representation of a function $F : \mathbb{R}^n \to \mathbb{R}^m$ in a box $\mathbf{x} = [z - r, z + r] \subseteq \mathbb{R}^n$ by a vector of polynomials $P(s)$ in $s = x - z$ of degree $d$ approximating the Taylor series, together with an error interval $\mathbf{e}$ such that

$$F(z + s) - P(s) \in \mathbf{e} \qquad \text{for all } s \in [-r, r]. \tag{22}$$

In exact arithmetic, $\mathbf{e} = O(r^{d+1})$, but in finite precision arithmetic, rounding errors also contribute to $\mathbf{e}$, and we have $\mathbf{e} = O(r^{d+1}) + O(\varepsilon)$, where $\varepsilon$ is the machine precision.

Taylor models can be computed recursively for any analytic function given by arithmetical expressions; explicit formulas for the arithmetic operations and some elementary fuctions are in the thesis by Makino [90]. Here we look only at addition and multiplication.

Hoefkens [43, p.23] defines (for simplicity, take in his formulas $x_0 = 0$ and the box $\mathbf{D} = [-r, r]$ symmetric around zero) the Taylor model $T_f = (P_f, 0, [-r, r], R_f)$ to mean

$$f(x) - P_f(x) \in R_f \quad \text{for all } x \in [-r, r],$$

and defines

$$T_{f+g} = (P_f + P_g, 0, [-r, r], R_f + R_g),$$
$$T_{fg} = (P_{fg}, 0, [-r, r], R_{fg}).$$

For details, [43] refers to MAKINO [90]. Her implementation chapter introduces on p. 108 order bound intervals $I^l$ for the homogeneous part of degree $l$, and gives explicit formulas for degree $l = 1$. Since degree 0 is trivial, we may conclude from this and her (4.7) that for order $n = 1$ and arbitrary factors $P_f = f_0 + f_1^T x$,

$$(fg)_0 = f_0 g_0, \quad (fg)_1 = f_0 g_1 + f_1 g_0,$$

$$R_{fg} = R_f R_g + R_f B_g + B_f R_g + |f_1|^T r \cdot |g_1|^T r[-1, 1],$$

where

$$B_f = f_0 + |f_1|^T r[-1, 1],$$

This is the optimal range for $P_f$, hence the best possible implementation. Similarly,

$$P_{af} = aP_f, \quad R_{af} = aR_f$$

in case the first factor is a constant.

These formulas are valid in exact arithmetic, but must be supplemented by safeguards to cope with rounding errors. Based on information from a lecture given at the SIAM Workshop on Validated Computing 2002 [123], what is implemented in COSY reduces for order $n = 1$ to something very close to

$$T_{f+g} = (P_h, 0, [-r, r], R_h),$$

where $P_h$ is defined by

$$h_0 \approx f_0 + g_0, \quad h_1 \approx f_1 + g_1,$$
$$R_h = R_f + R_g + (|h_0| + |h_1|^T r)[-\varepsilon, \varepsilon],$$

with upward rounded $|h_0| + |h_1|^T r$ (which is automatic if the rounding error interval is computed as a sum of individual intervals). Similarly,

$$T_{af} = (P_h, 0, [-r, r], R_h),$$

where $P_h$ is now defined by

$$h_0 \approx af_0, \quad h_1 \approx af_1,$$

and $R_h$ as before, and more complicated expressions for the product of two general functions.

# 11 Overestimation in Taylor forms

In problems where there is some dependence but little cancellation, Taylor forms give very litte accuracy beyond centered forms. For example

$$f(x) = \frac{1}{1-x} - \frac{1}{2-x}$$

evaluated naively at $\mathbf{x} = [-r, r]$ gives

$$f(\mathbf{x}) = \left[\frac{1}{1+r}, \frac{1}{1-r}\right] - \left[\frac{1}{2+r}, \frac{1}{2-r}\right] = \left[\frac{1-2r}{(1+r)(2-r)}, \frac{1+2r}{(1-r)(2+r)}\right]$$

with a radius of

$$\operatorname{rad} f(\mathbf{x}) = \frac{5}{4}r + O(r^3),$$

a centered form with slope

$$f[0, x] = \frac{1}{1-x} - \frac{1}{4-2x} \in \left[\frac{1}{1+r}, \frac{1}{1-r}\right] - \left[\frac{1}{4+2r}, \frac{1}{4-2r}\right] = \left[\frac{3}{4} - \frac{9}{8}r, \frac{3}{4} + \frac{9}{8}r\right] + O(r^2)$$

gives

$$f_c(\mathbf{x}) = \frac{1}{2} + f[0, \mathbf{x}]\mathbf{x} \in \left[\frac{1}{2} - \frac{3}{4}r - \frac{9}{8}r^2, \frac{1}{2} + \frac{3}{4}r + \frac{9}{8}r^2\right] + O(r^2)$$

with a radius of

$$\operatorname{rad} f_c(\mathbf{x}) = \frac{3}{4}r + \frac{9}{8}r^2 + O(r^3),$$

improving the naive evaluation by a factor of $0.6 + O(r)$. A Taylor expansion of arbitrary order

$$f(x) = \sum x^k - \sum 2^{-k-1}x^k = \frac{1}{2} + \frac{3}{4}x + \frac{7}{8}x^2 + \dots$$

gives an enclosure of radius $\frac{3}{4}r + \frac{7}{16}r^2 + O(r^3)$, with a marginal additional improvement factor of $1 - \frac{11}{12}r + O(r^2)$ only.

More generally, this is always the case when the centered form is already in its asymptotic regime where the quadratic approximation property is effective. Since the latter can be checked by monitoring the computable upper bounds for the overestimation derived in Theorem 8.1, one has a simple criterion for assessing when a higher order centered form (such as a Taylor model) may be useful. One simply compares the bounds from Theorem 8.1 with either the width of the enlosure or with the desired accuracy, and if it is too large, one repeats the computations at one order higher (and intersects). The process can be stopped if either the accuracy demands are met or the Hausdorff distance no longer decreases significantly (by a factor $\geq 2$, say).

# 12 Cancellation effects

For most arithmetic expressions, Taylor forms generate dependence. This can already be seen in simple examples such as (3) or

$$\frac{1}{1-x} = 1 + x + x^2 + \dots + \frac{x^{2k}}{1-x},$$

where the original expression has no dependence; in such cases, the interval evaluation always gives exact results, while Taylor forms produce overestimation.

However, much of the dependence is of a particularly simple kind, namely additive except in the remainder term. This has as a consequence that Taylor forms are frequently successful

in the computation of ranges of expressions involving significant cancellation, where traditional evaluation techniques such as centered forms suffer from severe overestimation due to dependent intervals. To see why this is so, consider the expression

$$f(\mathbf{x}) = \frac{1}{1+x} + \frac{1}{1-x} - \frac{2}{1-x^2} \tag{23}$$

which is identically zero. If we evaluate it in the interval

$$\mathbf{x} = [-r, r], \quad r < 1, \tag{24}$$

we find the naive interval enclosure

$$\begin{aligned} f(x) &= \frac{1}{[1-r, 1+r]} + \frac{1}{[1-r, 1+r]} - \frac{2}{[1-r^2, 1]} \\ &= \Big[\frac{2}{1+r} - \frac{2}{1-r^2}, \frac{2}{1-r^2} - 2\Big] = \Big[\frac{-2r}{1-r^2}, \frac{2r^2}{1-r^2}\Big], \end{aligned}$$

with a radius

$$\operatorname{rad} f(\mathbf{x}) = \frac{1}{2}\Big(\frac{2r^2}{1-r^2} + \frac{2r}{1-r^2}\Big) = \frac{r}{1-r}$$

of order $O(r)$, as predicted by general theory. A centered form using slopes

$$f[0, x] = \frac{f(x) - f(0)}{x - 0} = \frac{-1}{1+x} + \frac{1}{1-x} - \frac{2x}{1-x^2} \in \left[ -\frac{4r}{1-r^2}, \frac{4r}{1-r^2} \right]$$

gives the improved enclosure

$$f_c(\mathbf{x}) = f(0) + f[0, \mathbf{x}](\mathbf{x} - 0) = \left[\frac{-4r^2}{1-r^2}, \frac{4r^2}{1-r^2}\right]$$

of order $O(r^2)$, again as predicted by general theory. On the other hand, a Taylor form of odd order $d = 2k - 1$ proceeds by

$$\begin{aligned} f(x) &= \Big(1 - x + x^2 - \ldots + \frac{x^{2k}}{1+x}\Big) + \Big(1 + x + x^2 + \ldots + \frac{x^{2k}}{1-x}\Big) \\ &\quad -\Big(2 + 2x^2 + \ldots + \frac{2x^{2k}}{1-x^2}\Big) \\ &= \frac{x^{2k}}{1+x} + \frac{x^{2k}}{1-x} - \frac{2x^{2k}}{1-x^2} \\ &\in \frac{[0, r^{2k}]}{[1-r, 1+r]} + \frac{[0, r^{2k}]}{[1-r, 1+r]} - \frac{[0, 2r^{2k}]}{[1-r^2, 1]} = \left[\frac{-2r^{2k}}{1-r^2}, \frac{2r^{2k}}{1-r}\right], \end{aligned}$$

giving an enclosure of high order $O(r^{2k})$, and the even order case is similar. Thus overestimation due to cancellation effects can be efficiently suppressed by Taylor models. This is important in a number of applications where cancellations arise naturally. Examples include Lagrange interpolation, where the expression

$$f(x) = \sum f_i \prod_{k \neq i} \left( \frac{x - x_k}{x_i - x_k} \right)$$

typically involves severe cancellation (e.g., $f(x) \equiv x$ if $f_i = x_i$ for all $i$), computation of the even or odd part $\frac{1}{2}(f(x) \pm f(-x))$ of a function, interpolation by radial basis functions [12,

112], the evaluation of residual bounds in defect estimation [10], and normal form calculations for dynamical systems [46].

However, Taylor forms lose their superiority when no cancellation is present, or when some higher order terms in the Taylor expansion have a large coefficient. For example,

$$f(x) = (1+x)^4$$

is evaluated optimally by naive interval arithmetic,

$$f(\mathbf{x}) = [(1-r)^4, (1+r)^4], \quad \operatorname{rad} f(\mathbf{x}) = 4r + 4r^3,$$

whereas expansion and evaluation by the Horner scheme (which is naturally available from the recursive computation of Taylor forms) gives

$$f_T(\mathbf{x}) = 1 + \mathbf{x}(4 + \mathbf{x}(6 + \mathbf{x}(4 + \mathbf{x}))),$$

$$\operatorname{rad} f_T(\mathbf{x}) = r|4 + \mathbf{x}(6 + \mathbf{x}(4 + \mathbf{x}))| = 4r + 6r^2 + 4r^3 + r^4,$$

with an overestimation factor

$$p = \frac{6r^2 + r^4}{4r + 4r^3} = \frac{3}{2}r - \frac{5r^3}{4 + 4r^2}, \quad p \geq \frac{r}{4} \text{ for all } r.$$

The effect of a large Taylor coefficient can be seen from

$$f(x) = 1/(1 + x + 100x^2),$$

which has on $\mathbf{x} = [-0.1, 0.1]$ the range $[21/21, 400/399]$ (the maximum is attained at $x = -0.005$). Naive interval evaluation gives $[10/21, 10/9]$ with exact lower bound. The slope is

$$f[0, x] = -\frac{1 + 100x}{1 + x + 100x^2} \in \Big[-\frac{100}{9}, 10\Big],$$

giving

$$f_c(\mathbf{x}) = 1 + f[0, \mathbf{x}](\mathbf{x} - 0) = \Big[-\frac{1}{9}, \frac{19}{9}\Big],$$

which is worse, and Taylor forms are found to deteriorate with increasing order. In fact, the Taylor series diverges at the endpoints, since $f(x)$ has two complex conjugate poles of absolute values 0.1.

Even examples with much cancellation fail to give large improvements if the Taylor coefficients do not decay quickly. For example, let

$$f(x) = \frac{1}{n}\sum_{k=1}^{n} \sin(kx),$$

Naive interval arithmetic suffices for $\mathbf{x} = [-r, r]$, $r \leq \frac{\pi}{2n}$, the domain in which there is no overestimation. As $r$ increases, the terms with large $k$ oscillate more and more, giving rise to substantial cancellation for $r \geq \frac{2\pi}{n}$, but Taylor forms do not benefit much from it.

This suggests that during the recursive computation of Taylor forms, high order terms with large coefficients should be purged and moved into lower order terms (if interval coefficients are used) or into the remainder term (if only real coefficients are used).

# 13 Wrapping in Taylor models

Taylor models have been suggested by Berz, Makino and Hoefkens [9] as suitable techniques for a rigorous evaluation of the long time behavior of discrete and continuous dynamical systems. Some examples implemented in COSY INFINITY [24] are claimed to show a drastically reduced wrapping effect compared to traditional rigorous methods based on interval arithmetic and moving coordinate systems.

The wrapping strategy used, called *shrink wrapping*, is roughly outlined in Hoefkens [43, pp.151–152], and presented in more details by Berz in a lecture given at the SIAM Workshop on Validated Computing 2002 [123]. Intuitively, shrink wrapping means that after using the standard Taylor model for one time step, the box containing the set of initial conditions is enlarged enough to absorb the remainder box (which can then be reset to zero). Further steps are then calculated with the new, wider box and the old set of coefficients. To carry out this recipe, the error box is multiplied by the inverse of the linear coefficient matrix, and then added to the current initial box. (This is only an outline; the details are a little more complex.)

Thus, shrink wrapping is a nonlinear version of the parallelepiped method analyzed in Eijgenraam [35] and Nedialkov & Jackson [101], with known deficiencies for linear differential equations, that also should show up for nonlinear systems.

The publicly available material about wrapping in COSY does not seem to be enough to explain the little amount of wrapping reduction observed in the most interesting application, that to verified integration of asteroid dynamics in the solar system (Berz et al. [9]). An earlier paper Makino & Berz [92] treats only the rigorous enclosure of the force term. An implementation of their validated integrator is not publicly available.

In the paper [9], Section 3 refers to [90, 6] for details about the verified integration of ODEs through Taylor models. But the algorithm described in [90, 6] describes only a *single* time step, and fails for complicated problems like the solar system integrations. Thus it must be iterated for a number of time steps. But then (as we shall see) it suffers from severe wrapping already on simple linear problems.

It is essential that the additional techniques needed to stabilize the method are well documented, before the results can be trusted. To defend the validity of the reported verified integrations, formulas must be supplied that explain how precisely the new Taylor model is computed from the information in the old one, in sufficient detail that one can check that the recipe implies that the new Taylor model 'covers' the old one in the sense needed for rigor. To understand the absence of effects occurring in the parallelepiped method, one needs detailed performance comparisons for the linear case on examples with spectral properties for which it is known that the latter method shows exponential wrapping.

To claim a fully rigorous integration, full details about the rounding error control are needed, too: References to a documented rounding error analysis for IEEE arithmetic on which the implementation is based, or, if formulas not analyzed in the literature are used, to a mathematical proof that the error formulas used in the Taylor arithmetic implementation give rigorous results for IEEE arithmetic.

Since writing this, much of the missing information was disclosed in lectures given at the SIAM Workshop on Validated Computing 2002 [123] and at the Fields Institute Workshop on Validated Optimization [38]. Thus the prospects of soon having a fully rigorous and documented computer-assisted proof for the asteroid hitting problem are high.

In the following, we look at simple discrete dynamical systems for which an analysis of the wrapping performance of Taylor models (without additional wrapping safeguards) is possible. Note that the method of [90, 6], iterated over many time steps, is equivalent to such a discrete dynamical system, although with much more complex transition function than those considered here.

According to Jackson [48] (see also Gambill & Skeel [39], Neumaier [105], Kühn [77]), the wrapping effect occurs in its simplest form in discrete linear dynamical systems; thus we consider the iteration

$$y_{t+1} = A_t y_t + b_t \quad \text{for} \quad t = 0, 1, 2, \ldots, T-1. \tag{25}$$

Because of the linear structure of (25), we look at the special case where $y_0 = F_0(x)$ is a linear function of $x$; this corresponds to the most important situation where initial data in a known region are to be tracked over time. In this case, the iteration (25) ensures that all $y_t = F_t(x)$ are linear in $x$, too; therefore, all higher order Taylor coefficients vanish, and it is sufficient to consider Taylor models of the form

$$y_t = F_t(x) = c_t + B_t s + \tilde{e}_t, \quad x = z + s, \ |\tilde{e}_t| \le e_t, \tag{26}$$

where

$$c_t, e_t \in \mathbb{R}^n, \ B_t \in \mathbb{R}^{n \times m},$$

and inequalities and absolute values are interpreted componentwise. Note that we represent the error intervals in the form $[-e_t, e_t]$, reflecting the fact that, for the linear examples considered here, the error interval in actual Taylor model computations is nearly symmetric with respect to 0. This has the advantage that the analysis simplifies; but the results hold qualitatively also in the case of general error intervals.

If we insert (26) into (25) we see that

$$F_{t+1}(x) = A_t c_t + A_t B_t s + A_t \tilde{e}_t + b_t, \tag{27}$$

whence $c_{t+1} = A_t c_t + b_t, B_{t+1} = A_t B_t$ are the Taylor coefficients fo $F_{t+1}$. However, due to the limited precision of floating-point arithmetic, we can only compute approximations

$$c_{t+1} \approx A_t c_t + b_t, \quad B_{t+1} \approx A_t B_t \tag{28}$$

that are accurate within $O(\varepsilon)$. Therefore, we get for the error

$$\begin{aligned} \tilde{e}_{t+1} &= F_{t+1}(x) - c_{t+1} - B_{t+1} s \\ &= A_t c_t + b_t - c_{t+1} + (A_t B_t - B_{t+1}) s + A_t \tilde{e}_t, \end{aligned}$$

$$|\tilde{e}_{t+1}| \le |A_t c_t + b_t - c_{t+1}| + |A_t B_t - B_{t+1}| r + |A_t| e_t. \tag{29}$$

Therefore, $e_{t+1}$ must be chosen as a computable upper bound on the right-hand side of (29). In particular, we must have

$$e_{t+1} \geq |A_t| e_t, \tag{30}$$

and in typical cases where rounding errors occur in all components of $c_1$, we have

$$(e_1)_i \geq \delta > 0 \quad \text{for all } i, \tag{31}$$

with $\delta = O(\varepsilon)$. Now we specialize to the case where

$$A_t = A \quad \text{for all } t. \tag{32}$$

Basic results from the theory of nonnegative matrices (see, e.g., Berman & Plemmons [4] or Neumaier [104, Chapter 3.2]) imply that every nonnegative matrix $M$ has a nonnegative eigenvector $u$, whose associated eigenvalue is the spectral radius $\rho(M)$, the maximum of the absolute values of the eigenvalues of $M$. Therefore, there is a nonzero vector $u \geq 0$ such that

$$|A|u = qu, \quad q = \rho(|A|), \quad \|u\|_\infty = 1. \tag{33}$$

Now (31) implies $e_1 \geq \delta u$, and a simple induction argument using (30) and (33) gives

$$e_t \geq q^{t-1} \delta u \quad \text{for } t = 1, \ldots, T. \tag{34}$$

In particular, if $q > 1$, the errors grow exponentially, and the bounds remain below an acceptable level $e_{\max}$ only if

$$\log q \leq \Delta := \frac{\log(e_{\max}/\delta)}{T-1}. \tag{35}$$

For long time dynamics, $\Delta \ll 1$, hence $q$ is allowed to exceed 1 by only a small amount $\Delta + O(\Delta^2)$.

Many dynamical systems arising in practice are symplectic, and hence volume preserving. For volume preserving dynamics, the volume of the enclosing boxes is an immediate measure of the amount of overestimation involved, and hence an indicator of the severity of the wrapping effect. At any specific point $x$, the Taylor model (26) produces an enclosing box which is a translation of $[-e_t, e_t]$. By (34), this box has sides of length $\geq 2q^{t-1}\delta u_k$, and hence a volume of

$$\operatorname{vol} t \geq C q^{nt}, \quad C = \prod_{k=1}^{n} \frac{2\delta u_k}{q}. \tag{36}$$

Now the dynamical system (25) with constant matrices (32) is volume preserving iff $\det A = 1$, and since the determinant ist the product of the eigenvalues, there is at least one eigenvalue $\lambda$ of $A$ with $|\lambda| \geq 1$. Let $v$ be a corresponding left eigenvector, $v^T A = \lambda v^T \neq 0$. Then $0 < |v|^T u \leq |\lambda| \cdot |v|^T u = |\lambda v^T| u = |v^T A| u \leq |v|^T |A| u = |v|^T q u = q |v|^T u$, hence $q \geq 1$ unless $|v|^T u = 0$, which is possible only in degenerate situations.

Thus the spectral radius $q = \rho(|A|)$ figuring in the bound (36) is almost always at least one. Unfortunately, it is usually significantly larger, implying a severe wrapping effect. For example, for 2-dimensional rotations, which are volume preserving, we have

$$A = \begin{pmatrix} \cos\alpha & \sin\alpha \\ -\sin\alpha & \cos\alpha \end{pmatrix}, \quad q = \rho(|A|) = \cos\alpha + \sin\alpha,$$

and for $\alpha = \pi/4$, we get $q = \sqrt{2}$.

We conclude that Taylor models by themselves do not cope adequately with the wrapping effect. This can also been seen simpler by noting that in the limit where the input width goes to zero, Taylor models reduce to centered interval arithmetic, which is inferior to standard interval arithmetic in higher order terms (consider, e.g., squaring $1 + [-h, h]$), and already the latter leads to exponential growth of rounding errors in wrapping-prone computations.

Therefore, to cope successfully with problems involving dynamical systems, Taylor models (and other Taylor forms) need to be combined with special wrapping reduction techniques such as those advocated in Jackson [48, 49, 50], Lohner [83], Gambill & Skeel [39], Alvarado & Wang [1, 130], Barbarosie [3], Stewart [125], Kühn [77]. Among these, the zonotope techniques of Kühn hold the best promise.

Two recent papers analyzing the wrapping effect are Lohner [89] and Nedialkov & Jackson [101]. For alternative techniques in verifying dynamical systems see Chernousko [18], Janssen et al. [52] and Milanese et al. [94].

The fact that the computations with COSY INFINITY reported in [9] show very little wrapping effect is apparently due to the incorporation of shrink wrapping. For Taylor models of order 1, shrink wrapping can be viewed as a simple special case of the zonotope techniques of Kühn [77] for zonotopes of the form $Z = \{(B, I)\tilde{u} \mid \tilde{u} \in \mathbf{u}\}$ with square $B \in \mathbb{R}^{n \times n}$. For higher orders, it then is a nonlinear version of this, with a polynomial operator in place of $B$.

# 14 Two simple test problems for verified ODE solvers

**Example 1.** The stable linear system

$$\begin{aligned} y_1' &= y_1 - 3y_2 \\ y_2' &= 3y_1 - 9y_2 \\ y_1(0) &= 1, y_2(0) = -1 \end{aligned}$$

has the solution

$$y_1(t) = 1.5 - 0.5e^{-8t}, \quad y_2(t) = 0.5 - 1.5e^{-8t}.$$

Rudolf Lohner (personal communication) calculated the solution with AWA, using order $p = 20$ and constant step size $h = 0.0625$ on an Athlon MP1900+ with 1.6GHz. The computation of 160 time steps from $t = 0$ to $t = 10$ took 0.08 seconds, and produced the final enclosure

$$y(10) \in \begin{pmatrix} [1.49999999999998, 1.50000000000002] \\ [0.499999999999995, 0.500000000000006] \end{pmatrix},$$

which was reached at about $t = 4.75$ and did not change afterwards. (It remained constant for all times $10 \le t \le 1000$. A version with step size control lead to very slight growth with time, reaching at $t = 10^6$ intervals with diameter of about $5 \cdot 10^{-9}$.)

It would be interesting to see how Makino's COSY-VI (which is not publicly available) performs on this problem.

**Example 2.** For the dynamical system

$$\dot{y} = F(y) := \begin{pmatrix} 9.9y_1 - 7.6y_2 + 7.6 \\ 12.6y_1 - 9.9y_2 + 9.9 + y_1^3/7.6 \end{pmatrix}, \tag{37}$$

the quantity $c := \frac{1}{2}(y_1^2 - 2.25)^2 + (9.9y_1 - 7.6y_2 + 7.6)^2$ is conserved. There are two stable fixed points with $c = 0$ at $y = \binom{\pm 1.5}{1 \pm 297/152}$ and an unstable fixed point with $c = 81/32$ at $y^* = \binom{0}{1}$. For $0 \le c < 81/32$, there are two orbits, for $c = 81/32$ there are three, and for $c > 81/32$ there is a single orbit. All orbits are periodic, so that the system remains bounded for all times.

$$F'(y) = \begin{pmatrix} 9.9 & -7.6 \\ 12.6 + 3y_1^2/7.6 & -9.9 \end{pmatrix}$$

has trace zero, hence the system is volume preserving. Since $\det F'(y) = 3y_1^2 - 2.25$, the eigenvalues of the Jacobian are real if $|y_1| \le \frac{1}{2}\sqrt{3} \approx 0.866$, and purely imaginary otherwise. Thus the dynamics is locally unstable within the slab defined by $|y_1| \le \frac{1}{2}\sqrt{3}$, and every nontrivial orbit intersecting $y_2 = 1$ goes through two unstable phases per period; cf. Figure 1.

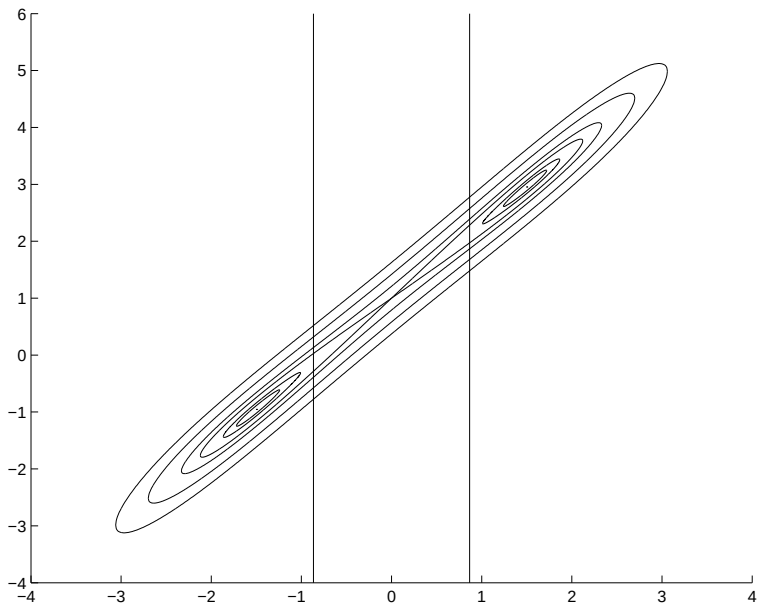


Figure 1: Phase diagram and region of local instability (between the two lines)

This makes it interesting to look at what happens for trajectories starting at a point with $y_2 = 1$ and various small $y_1 \neq 0$. Rudolf Lohner calculated on the same machine as above the solution with AWA, using order $p = 20$ and adaptive step size two cases. For $y_1(0) = 2^{-16}$, AWA breaks down after 1566 time steps and 2.6 seconds time at $t = 33.91014270298183$ with

$$y(t) \in \begin{pmatrix} [-196.199244777380, 196.226298193513] \\ [6039.01251175114, 6041.04241329249] \end{pmatrix}.$$

The last step with an absolute accuracy of $< 0.01$ was at $t' = 30.68380898237228$ (i.e., after

roughly one period) with

$$y(t') \in \begin{pmatrix} [-4.21196806856650 \cdot 10^{-3}, 4.37969298878639 \cdot 10^{-3}] \\ [0.997316960688021, 1.00285014334261] \end{pmatrix};$$

$t'' = 29.36669719219208$ was the first time where the unstable fixed point $\binom{0}{1}$ was contained in the enclosure.

For $y_1(0) = 2^{-8}$, AWA breaks down after 9943 time steps and 16.2 second time at $t = 322.1113151842728$ with

$$y(t) \in \begin{pmatrix} [-205.835463419725, 203.661675220156] \\ [-6639.98576998417, 6638.78554475260] \end{pmatrix}.$$

The last step with an absolute accuracy of $< 0.01$ was at $t' = 318.3003144860268$ (i.e., after about 20.5 periods) with

$$y(t') \in \begin{pmatrix} [-5.18350510450575 \cdot 10^{-2}, -4.29950341365378 \cdot 10^{-2}] \\ [0.943970694860419, 0.953744955892377] \end{pmatrix};$$

$t'' = 321.8574418425560$ was the first time where the unstable fixed point $\binom{0}{1}$ was contained in the enclosure.

Again, it would be interesting to see the behavior of COSY-VI on this problem.

We can analyze what may happen for Taylor models without wrapping precautions, based on the linear analysis given before. Very close to the unstable fixed point, the trajectory changes only very little and hence can be approximated over fairly long times by the linear dynamical system

$$\dot{y} = B(y - y^*), \quad B = \begin{pmatrix} 9.9 & -7.6 \\ 12.6 & -9.9 \end{pmatrix} \tag{38}$$

Using the spectral factorization

$$B = SDS^{-1}, \quad S = \begin{pmatrix} 1.9 & -2.0 \\ 2.1 & -3.0 \end{pmatrix}, \quad D = \begin{pmatrix} 1.5 & 0 \\ 0 & -1.5 \end{pmatrix}, \quad S^{-1} = \frac{1}{3}\begin{pmatrix} 6.0 & -4.0 \\ 4.2 & -3.8 \end{pmatrix},$$

it is easy to see that

$$\exp\left(\frac{2}{3}\log 2 \cdot B\right) = S \begin{pmatrix} 2.0 & 0 \\ 0 & 0.5 \end{pmatrix} S^{-1} = \begin{pmatrix} 6.2 & -3.8 \\ 6.3 & -3.7 \end{pmatrix}. \tag{39}$$

Therefore, if we proceed in steps of length $h = \frac{2}{3}\log 2$, we obtain for $y_t = y(ht)$ the discrete dynamical system

$$y_{t+1} = Ay_t + b, \quad t = 0, 1, 2, \ldots \tag{40}$$

with

$$A = \begin{pmatrix} 6.2 & -3.8 \\ 6.3 & -3.7 \end{pmatrix}, \quad b = \begin{pmatrix} 3.8 \\ 4.7 \end{pmatrix}.$$

The system (40) has the fixed point $y^* = \binom{0}{1}$, and from (39) one finds (in the $\infty$-norm)

$$\|y_t - y^*\| \le \|A^t\|\|y_0 - y^*\| \le 2^t\|S\|\|S^{-1}\|\|y_0 - y^*\| = 17 \cdot 2^t\|y_0 - y^*\|.$$

In particular, for the uncertain initial conditions

$$y_0 \in \begin{pmatrix} [10^{-15}, 3 \cdot 10^{-15}] \\ 1 \end{pmatrix}, \tag{41}$$

we have $\|y_t - y^*\| < 0.002$ for $t \le 35$, whence (38) and hence (40) is a good approximation to (37) for the first 35 time steps, i.e. for continuous time up to about $y(16)$.

Since the spectral radius $\rho(|A|)$ has the value 10, running the recurrence (40) in Taylor mode increases the width of the error interval by roughly a factor of 10 in each step, making the enclosure useless long before the linear approximation breaks down. We see again that Taylor arithmetic has no intrinsic capacity for avoiding the wrapping effect, although it may reduce the part of wrapping caused by nonlinearities. Thus it needs to be combined with wrapping reducing strategies.

In such a combination, Taylor arithmetic may make many problems tractable that used to defy a rigorous treatment until now.

# 15 Conclusions

1. The various versions of Taylor arithmetic constitute a significant enhancement of the toolkit of interval analysis techniques. Indeed, interval coefficient versions were used by mathematical physicists to prove estimates important for computer-assisted proofs, and floating-point coefficient versions were used by Berz and his group to verify solutions of celestial mechanics problems that so far defied interval techniques.

Berz and his group also used Taylor models for applications to multivariate integration over a box, differential algebraic equations, and other problems that have not been discussed before in the interval literature.

2. The currently implemented versions of Taylor arithmetic that do not attempt to compute the exact range of the quadratic term, enclose ranges to second order only, as other centered forms.

However, in problems where in real arithmetic substantial cancellation of leading digits occurs, Taylor arithmetic may drastically reduce overestimation over intervals narrow enough such that the remainder intervals remain sufficiently small. These are sometimes quite small intervals and sometimes quite wide ones, depending on the problem. If dependent intervals are present but without the cancellation structure, gains from a Taylor arithmetic are slight, and the much higher cost and storage does not justify their use.

3. Taylor arithmetic in itself does not eliminate the wrapping effect. It may drastically reduce that part of the wrapping effect due to nonlinearities, since the nonlinear dependence on initial conditions is taken into account to a large extent, while methods like Lohner's AWA incur here additional wrapping from the need to enclose bended boxes into parallelepipeds.

However, the part of wrapping incurred by the error term, that is already present for linear systems and that may even magnify rounding errors exponentially, is not addressed at all by Taylor arithmetic. It must be combatted by techniques analogous to those used in traditional interval differential equation solvers.

Shrink wrapping, the nonlinear generalization of the parallelepiped method, is a good remedy for problems whose Jacobians have no eigenvalues with significantly differing real parts, or where drastic phase space volume reductions compensate the wrapping. This is apparently the case for the asteroid problem and (for some time) for the Lorenz attractor, but it excludes already simple 2-dimensional Hamiltonian dynamical systems with a hyperbolic fixed point, which are very benign from an analytic point of view.

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