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Efficient Control of the Dependency Problem Based on Taylor Model Methods

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Abstract. It is shown how the Taylor Model approach allows the rigorous description of functional dependencies with far-reaching control of the dependency problem. The amount of overestimation decreases with a high power of the interval over which the information is required, at a computational expense that increases rather moderately with the dimensionality of the problem. This leads to the possibility of treating even cases with a very significant dependency problem that are intractable using conventional methods.

1. Introduction

A common task in the use of modern verified methods is the determination of rigorous upper and lower bounds of a function; one example is the range bounding subproblem of global optimization. The commonly used interval approach has excelled in solving this problem elegantly from both a formal and an implementational viewpoint. However, there are situations where the method has limitations for extended or complicated calculations because of the dependency problem, which is characterized by a cancellation of various sub-parts of the function that cannot be detected by direct use of interval methods. This effect often leads to pessimism and sometimes even drastic overestimation of range enclosure. Furthermore, the sharpness of intervals resulting from calculations typically scales linearly with the sharpness of the initial discretization intervals. For complicated problems, and in particular higher dimensions, this sometimes significantly limits the sharpness of the resulting answer that can be obtained.

In the following, we study some applications of the Taylor model approach that allows us to obtain fully mathematically rigorous range enclosures while largely avoiding many of the limitations of the conventional interval method. The method is based on the inductive local modelling of functional dependencies by a polynomial with a rigorous remainder bound, and as such represents a hybrid between formula manipulation, interval methods, and methods of computational differentiation [6], [9]. In all cases, the computational expense scales only linearly with the expense of the underlying function, resulting in the ability to treat rather large and complicated computational problems.

2. Properties of the Taylor Model Method

In [7], [10], a method has been introduced that allows the rigorous modeling of functional dependencies by a local inclusion into a Taylor polynomial with floating point coefficients plus an interval. Specifically, let f be $C^{(n+1)}$ on $D_f \subset R^v$, and $\vec{B} = [a_1, b_1] \times \cdots \times [a_v, b_v] \subset D_f$ an interval box containing the point $\vec{x}_0$. Let T be the Taylor polynomial of f around the point $\vec{x}_0$. We call the interval I an n-th order remainder bound of f on $\vec{B}$ if

$$f(\vec{x}) - T(\vec{x}) \in I \quad \text{for all} \quad \vec{x} \in \vec{B}.$$

In this case, we call the pair (T, I) an n-th order Taylor Model of f on $\vec{B}$. It is clear that a given function f can have many different Taylor models, as with (T, I), also $(T, \bar{I})$ with $\bar{I} \supset I$ is a Taylor model. Furthermore, we see that low-order polynomials have trivial remainder bounds; since every polynomial of order not exceeding n agrees with its n-th order Taylor polynomial, the interval $[0, 0]$ is a remainder bound. For practical purposes, it is important that if the original interval box $\vec{B}$ decreases in size, then according to the various formulas of the Taylor remainder, the remainder bounds can decrease in size with a power of $n+1$ and hence become small quickly.

The strategy of both the interval method and the methods of computational differentiation is to extract information for complicated functional dependencies from those of simpler functional dependencies, and rules to combine them. In practice, one begins with the identity function, and derives rules how to extract bounds or derivatives of sums, products, and intrinsics from those of the arguments.

In [7], [10], it has been shown how it is possible to build up Taylor models of complicated functions from the known Taylor model of their pieces, starting from the identity function which has zero remainder bound, and then proceeding inductively. For this purpose, it is necessary to study to what extent it is possible to define arithmetic operations $\oplus$, $\odot$, and others on Taylor models that preserve the respective operations in the underlying function spaces. Thus it is necessary to craft new adjoint operations on Taylor models that make the diagram

$$\begin{array}{ccc} f, g \in C^{n+1} & \xrightarrow{\subset} & (T_f, I_f), (T_g, I_g) \\ \Big\downarrow * & & \Big\downarrow \circledast \\ f * g & \xrightarrow[\subset]{} & (T_f, I_f) \circledast (T_g, I_g) \end{array} \tag{2.1}$$

commute.

For practical purposes, it is worthwhile to assess the computational expense of operations on Taylor models, since their data types are obviously more complicated

Table 1. The number of coefficients $N(n, v)$ of a polynomial of order n in v variables.

Order	Variables 1	2	3	4	5	6	7	8
1	2	3	4	5	6	7	8	9
2	3	6	10	15	21	28	36	45
3	4	10	20	35	56	84	120	165
4	5	15	35	70	126	210	330	495
5	6	21	56	126	252	462	792	1,287
6	7	28	84	210	462	924	1,716	3,003
7	8	36	120	330	792	1,716	3,432	6,435
8	9	45	165	495	1,287	3,003	6,435	12,870
9	10	55	220	715	2,002	5,005	11,440	24,310
10	11	66	286	1,001	3,003	8,008	19,448	43,757

than mere intervals. Specifically, it has been shown in [8] that the number of coefficients of a polynomial of order n in v variables is given by

$$N(n, v) = \binom{n+v}{v} = \frac{(n+v)!}{n! \cdot v!}. \tag{2.2}$$

As can be seen from Table 1, for values of n and v in the middle of those shown, an increase of the order by one results in roughly a doubling of the number of coefficients. Likewise, an increase in the dimensionality by one also results roughly in a doubling of the number of coefficients. This is in stark contrast to common scanning techniques, where each new dimension entails a multiplication of the previous effort by the number of support points used per dimension.

From the aspect of implementation, besides the use of elementary interval tools, the method requires efficient tools for high-order multivariate Taylor operations [1], [4]. In our implementation, we use the approach outlined in [3], which has a particularly sophisticated addressing scheme that reduces the amount of effort for bookkeeping to a small fraction of what is needed for floating point operations and fully supports sparsity of the polynomials. It has been used for more than a decade in Beam Physics [2] by hundreds of users of the code COSY INFINITY.

Altogether, the Taylor model approach has the following important properties:

- The width of the remainder term, and hence the sharpness of the range enclosure, scales with the $(n+1)$-st order of the domain interval and hence decreases quickly with order. Any dependency problem of the task manifests itself only in the remainder term, where its significance is substantially suppressed according to the overall size of the remainder term.

- The computational expense increases only moderately with order, allowing the computation of sharp range enclosures even for complicated functional dependencies with significant dependency problem.
- The computational expense of higher dimensions increases only very moderately, significantly reducing the “curse of dimensionality.”

In the following sections, we present some examples and applications to show the practical use and power of the method.

3. A Multidimensional Function

As a first example addressing the dependency problem, we study a somewhat randomly chosen function of three variables

$$\begin{aligned} f(x_1, x_2, x_3) \;=\; & \frac{4\tan(3x_2)}{3x_1 + x_1\sqrt{\dfrac{6x_1}{-7(x_1-8)}}} - 120 - 2x_1 \\ & - 7x_3(1+2x_2) - \sinh\left(0.5 + \frac{6x_2}{8x_2+7}\right) + \frac{(3x_2+13)^2}{3x_3} \\ & - 20x_3(2x_3-5) + \frac{5x_1\tanh(0.9x_3)}{\sqrt{5x_2}} - 20x_2\sin(3x_3). \end{aligned}$$

There are nine terms contributing to the result, each of which consists of not fully trivial arithmetic. Since each variable appears several times, terms depend on one another. Hence, a certain amount of blow up due to the dependency problem is to be expected in conventional interval arithmetic.

To study the effect, we ask for the range enclosure of the function over a three dimensional box centered around $(2, 1, 1)$ with width of 0.1 in each dimension, so that $x_1 \in [1.95, 2.05]$, $x_2 \in [0.95, 1.05]$, and $x_3 \in [0.95, 1.05]$.

The non-verified range enclosure estimate of the function obtained by scanning in real numbers at $11 \times 11 \times 11$ equidistant points is

```
[ -2.31165715, 1.78168226].
```

When the function is evaluated with the above domain intervals in naive interval arithmetic, the range enclosure is

```
[-16.36393303, 16.09747985],
```

which is almost ten times wider than the range enclosure estimated via naive scanning.

We now evaluate the function in Taylor model arithmetic around the reference point $\vec{x}_0 = (2, 1, 1)$. Table 2 provides a summary of the range enclosure intervals of the function obtained through interval methods with various numbers of equidistant subdivisions of the interval box as well as with Taylor model computation as a

Table 2. Range enclosure of the three dimensional function.

Real Number Rastering	
Sampling Points	Range Enclosure
$11 \times 11 \times 11$	[-2.31165, 1.78168]

Interval Method				
Sub-division	Width in Subdivisions			Total Range Enclosure
	Maximum	Minimum	Average	
1^3	32.46141	32.46141	32.46141	[-16.36393,16.09747]
2^3	16.63312	15.81953	16.22488	[-9.22796, 9.04085]
4^3	8.42057	7.80824	8.11117	[-5.73777, 5.43391]
8^3	4.23647	3.87888	4.05529	[-4.01617, 3.61282]
16^3	2.12481	1.93314	2.02757	[-3.16171, 2.69842]
32^3	1.06405	0.96500	1.01377	[-2.73613, 2.24033]
64^3	0.53243	0.48222	0.50688	[-2.52387, 2.01107]

Taylor Model Method			
Order	Terms	Remainder Bound	Total Range Enclosure
1	4	[-.39140 ,0.72524]	[-2.80268, 2.35080]
2	10	[-.33950E-01,0.33940E-01]	[-2.48316, 1.84826]
3	20	[-.10202E-02,0.16096E-02]	[-2.47884, 1.84454]
4	35	[-.84132E-04,0.84028E-04]	[-2.47871, 1.84429]
5	56	[-.24107E-05,0.43833E-05]	[-2.47866, 1.84424]
6	84	[-.33555E-06,0.33431E-06]	[-2.47866, 1.84424]
7	120	[-.16319E-07,0.20518E-07]	[-2.47866, 1.84424]
8	165	[-.24246E-08,0.24107E-08]	[-2.47866, 1.84424]
9	220	[-.17219E-09,0.17367E-09]	[-2.47866, 1.84424]
10	286	[-.23138E-10,0.22986E-10]	[-2.47866, 1.84424]
11	364	[-.19280E-11,0.18210E-11]	[-2.47866, 1.84424]
12	455	[-.24243E-12,0.24077E-12]	[-2.47866, 1.84424]
13	560	[-.21634E-13,0.20126E-13]	[-2.47866, 1.84424]
14	680	[-.26147E-14,0.25966E-14]	[-2.47866, 1.84424]
15	816	[-.24172E-15,0.22428E-15]	[-2.47866, 1.84424]

function of the order. Table 2 also lists the number of coefficients of the polynomial in the given order, which can serve as an estimate of the computational expense for the computation of the range enclosure. While the number of terms of polynomial increases moderately with order, the width of remainder range enclosure interval

Table 3. Output of the fifth order Taylor model of the three dimensional function, which consists of the Taylor coefficients, the domain information and the remainder bound.

```
 RDA VARIABLE:   NO=   5, NV=     3
 I  COEFFICIENT          EXPONENTS   I  COEFFICIENT          EXPONENTS
 1  -.3928616701165386     0 0 0    24  -3.675895416398908     0 4 0
 2  -.3539134581708554     1 0 0    25  0.3674633576464710     1 2 1
 3   15.04043477798914     0 1 0    26  -.6124389294107850     0 3 1
 4  -24.97397896319208     0 0 1    27  0.3158558645500195     1 1 2
 5  -.2240287293503141E-01 2 0 0    28   2.526216203174971     0 2 2
 6  -1.754174272159207     1 1 0    29  0.1426707720152316     1 0 3
 7   3.585368696366333     0 2 0    30  -121.2419954660553     0 1 3
 8  0.9799022870572560     1 0 1    31   75.96490653676481     0 0 4
 9   12.41964750896948     0 1 1    32  0.2858741733383875E-02 5 0 0
10   56.77071060052130     0 0 2    33  0.1222499625765752     4 1 0
11  0.1132471389197260E-01 3 0 0    34  0.1039934394699180     3 2 0
12  0.4810657908262914     2 1 0    35   1.531172592862926     2 3 0
13   1.008315244119392     1 2 0    36   2.958604600578060     1 4 0
14   4.453227097958014     0 3 0    37   20.81296131572292     0 5 0
15  -.4899511435286280     1 1 1    38  -.3062194647053925     1 3 1
16  -2.265073284707058     0 2 1    39  0.5358840632344369     0 4 1
17  -.6317117291000389     1 0 2    40  -.2368918984125146     1 2 2
18   45.33251245448809     0 1 2    41  0.3948198306875244     0 3 2
19  -174.1473164833430     0 0 3    42  -.7133538600761581E-01 1 1 3
20  -.5693089033022302E-02 4 0 0    43  -2.892996920988576     0 2 3
21  -.2431800805245985     3 1 0    44  0.7858687373626551E-01 1 0 4
22  -.2057227964207444     2 2 0    45   22.39581258222270     0 1 4
23  -3.534855720652786     1 3 0    46  -45.38843038572212     0 0 5
--------------------------------    --------------------------------

VAR    REFERENCE POINT                      DOMAIN INTERVAL
  1  2.000000000000000     [ 1.950000000000000  , 2.050000000000000  ]
  2  1.000000000000000     [0.9500000000000000  , 1.050000000000000  ]
  3  1.000000000000000     [0.9500000000000000  , 1.050000000000000  ]
                 REMAINDER BOUND INTERVAL
  R     [-.2410738165297327E-05,0.4383393685666131E-05]
*******************************************************
```

drops down sharply as expected, reaching ten digits of accuracy with fewer than 300 polynomial coefficients.

To illustrate the Taylor model method in more detail, in Table 3 we list the actual fifth order Taylor model obtained with the code COSY, providing all expansion coefficients as well as the domain information and the bound for the remainder.

4. A Highly Complicated Six-Dimensional Function

The next example is a range enclosure of a normal form invariant function [5] of a dynamical system. Specifically, the function is a six dimensional polynomial of degree roughly 200 that is always rather near to zero in value, while having a large number of local minima and maxima. Because of the many cancellations and the dimensionality, it thus represents a substantial challenge for verified bounding tools. We study the determination of a range enclosure of the function on the six dimensional box

$$\vec{B} = [0.04, 0.06] \times [0.04, 0.06] \times [0.04, 0.06] \times [0.04, 0.06] \\ \times [0.04, 0.06] \times [0.04, 0.06],$$

which has width of 0.02 in each dimension and center point $\vec{x}_0 = \overrightarrow{0.05}$. The value of the function at the reference point is

$$f(\vec{x}_0) = 0.6976700784514303 \times 10^{-5},$$

and a non-verified range enclosure is obtained by scanning in real numbers at a total of 1729 points in the whole domain, which consist of 3^6 equidistant points including boundary points, and 1000 randomly chosen points, as

```
[-0.31211856E-05, 0.42124293E-04].
```

Using naive interval arithmetic covering the whole domain by one interval box gives a mathematically rigorous range enclosure of

```
[ -4.47134 , 4.80774 ],
```

which exhibits a blow-up of about six orders of magnitude due to the dependency problem of the function.

Dividing the domain in question into smaller interval boxes, we expect to obtain a narrower range enclosure. Table 4 shows range enclosures using successively smaller domain interval boxes at various locations. Only the smallest boxes yield a range enclosure of a size comparable to those obtained by the scanning estimate. However, to cover the entire domain in this fashion would requires 10^{24} small interval boxes, showing the practical limitations of the interval approach for this problem.

We next study the bounding problem for the normal form invariant function with the Taylor model approach. The entire domain interval is covered with one Taylor model without subdivision. To obtain the required sharpness, the order of the Taylor model is increased. Table 5 shows the range enclosure computed with various orders. Already at order six, the total range enclosure is within a factor of two of the non-verified range enclosure obtained by scanning.

Table 5 also shows the number of terms of the occurring polynomials, which are very moderate compared to the number of divisions necessary for a comparable interval evaluation. Indeed, the naive interval method would require roughly 10^{20} more computational effort than the Taylor model approach.

Table 4. Range enclosures of a normal form invariant function via interval methods.

Interval Method		
Domain Interval Box	Range Enclosure	Width
[0.040000, 0.060000]^6	[-4.47134 , 4.80774]	9.27908
[0.040000, 0.042000]^6	[-0.281964E-02, 0.424588E-02]	0.70655E-02
[0.040000, 0.040200]^6	[-0.311303E-03, 0.327498E-03]	0.63880E-03
[0.040000, 0.040020]^6	[-0.304618E-04, 0.329529E-04]	0.63414E-04
[0.040000, 0.040002]^6	[-0.199253E-05, 0.434435E-05]	0.63368E-05
[0.049000, 0.051000]^6	[-0.544365E-02, 0.100332E-01]	0.15476E-01
[0.049900, 0.050100]^6	[-0.697752E-03, 0.762484E-03]	0.14602E-02
[0.049990, 0.050010]^6	[-0.657704E-04, 0.802314E-04]	0.14600E-03
[0.049999, 0.050001]^6	[-0.320844E-06, 0.142793E-04]	0.14600E-04
[0.058000, 0.060000]^6	[-0.133070E-01, 0.265293E-01]	0.39836E-01
[0.059800, 0.060000]^6	[-0.160977E-02, 0.188511E-02]	0.34948E-02
[0.059980, 0.060000]^6	[-0.144312E-03, 0.207897E-03]	0.35220E-03
[0.059998, 0.060000]^6	[0.131290E-04, 0.483782E-04]	0.35249E-04

Table 5. Range enclosures of a normal form invariant function via Taylor model methods.

Taylor Model Method			
Order	Terms	Remainder Bound	Total Range Enclosure
6	924	[-0.53585E-05,0.53588E-05]	[-0.3466E-04,0.5358E-04]
7	1716	[-0.83873E-06,0.83884E-06]	[-0.3016E-04,0.4902E-04]
8	3003	[-0.12321E-06,0.12321E-06]	[-0.2945E-04,0.4831E-04]

5. Many Body Dynamics

As the final example, we study the problem of many body dynamics, in which an ensemble of particles interact via two-body forces. The many body dynamics problem occurs in many disciplines including plasma physics, beam physics, and galaxy dynamics (see Figure 1). For the specific case of Coulomb fields, the force on a test particle is given by

$$\vec{F}(\vec{x_j}) = \sum_{\substack{i = 1, \ldots, N \\ i \neq j}} \frac{q_j q_i \cdot (\vec{x_j} - \vec{x_i})}{|\vec{x_j} - \vec{x_i}|^3},$$

where $\vec{x_i}$ and q_i are position and charge of the i-th particle of the ensemble. The study of the dynamics requires the solution of the equations of motion for the particles, which in principle can be done with a variety of verified integration methods. A necessary part of such calculations is the computation of the force at the position $\vec{x_j}$.

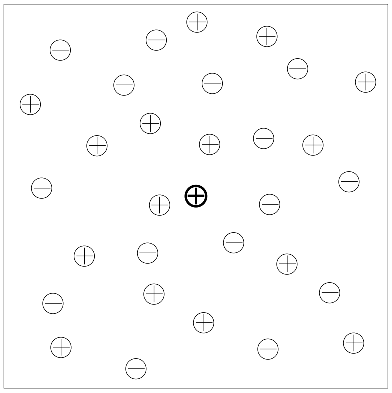

Figure 1. Test particle in many particle system.

Using verified methods after some time evaluation, the $\vec{x}_j$ themselves will be given by interval boxes. Hence it is desirable to determine a rigorous and tight enclosure of the force $\vec{F}$ over this interval box.

We now study this computation of forces using interval arithmetic and Taylor model arithmetic for many body systems. To assess the quality of the enclosures, we choose randomly distributed $\vec{x}_i \in [-1, 1]^3$ and $q_i \in \{-1 / N, 1 / N\}$ for different values of N, which correspond to the simulation of a plasma or beam by more and more sub-particles.

In this situation, if $\vec{x}_j$ is chosen to be a box around the origin, as N increases, the force at $\vec{x}_j$ decreases with N, as the forces have a tendency to cancel each other more and more. Specifically, we choose $\vec{x}_j \in [-0.001, 0.001]^3$ and determine a range enclosure for the resulting force on the box. Figure 2 shows the range enclosure of the force for the values of $\vec{x}_j$ in this interval, using non-verified rastering, interval computation, and computation using Taylor models. The rastering clearly shows the effect of a decrease of the force as the number of particles increases. On the other hand, the interval estimate of the force shows no decrease with the number of particles, but instead asymptotically approaches a constant, non-zero value. The Taylor model bounding avoids the dependency problem arising from the repeated occurrence of $\vec{x}_j$ in each term and yields range enclosure with the proper asymptotics that in fact have a tightness very similar to that of the non-verified bounding.

Acknowledgements

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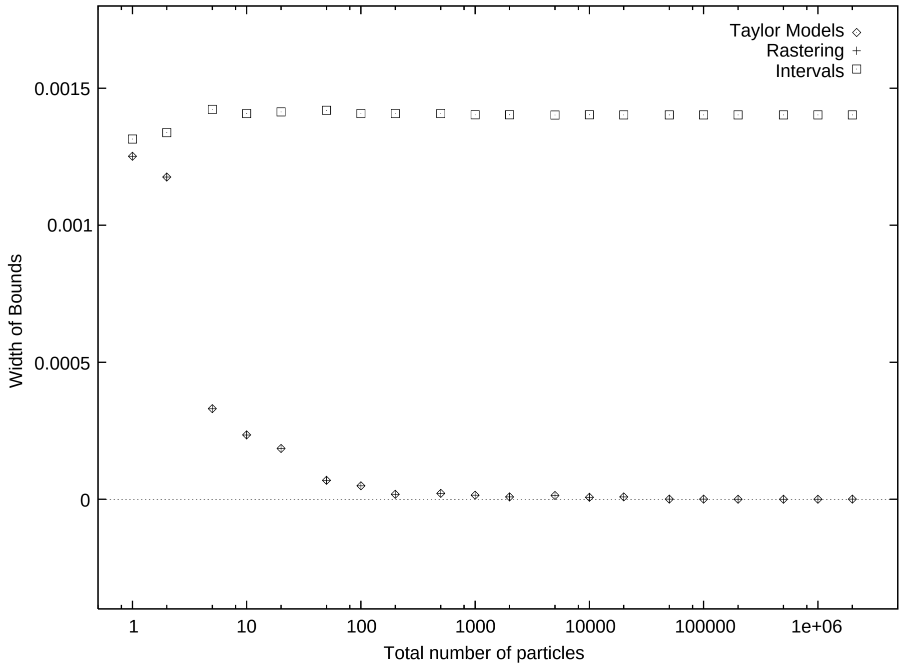

Figure 2. Range enclosure estimate of force on test particle within interval box.

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