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Optimal correction and design parameter search by modern methods of rigorous global optimization[☆]

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ABSTRACT

Frequently the design of schemes for correction of aberrations or the determination of possible operating ranges for beamlines and cells in synchrotrons exhibit multitudes of possibilities for their correction, usually appearing in disconnected regions of parameter space which cannot be directly qualified by analytical means. In such cases, frequently an abundance of optimization runs are carried out, each of which determines a local minimum depending on the specific chosen initial conditions. Practical solutions are then obtained through an often extended interplay of experienced manual adjustment of certain suitable parameters and local searches by varying other parameters.

However, in a formal sense this problem can be viewed as a global optimization problem, i.e. the determination of all solutions within a certain range of parameters that lead to a specific optimum. For example, it may be of interest to find all possible settings of multiple quadrupoles that can achieve imaging; or to find ahead of time all possible settings that achieve a particular tune; or to find all possible manners to adjust nonlinear parameters to achieve correction of high order aberrations. These tasks can easily be phrased in terms of such an optimization problem; but while mathematically this formulation is often straightforward, it has been common belief that it is of limited practical value since the resulting optimization problem cannot usually be solved.

However, recent significant advances in modern methods of rigorous global optimization make these methods feasible for optics design for the first time. The key ideas of the method lie in an interplay of rigorous local underestimators of the objective functions, and by using the underestimators to rigorously iteratively eliminate regions that lie above already known upper bounds of the minima, in what is commonly known as a branch-and-bound approach.

Recent enhancements of the Differential Algebraic methods used in particle optics for the computation of aberrations allow the determination of particularly sharp underestimators for large regions. As a consequence, the subsequent progressive pruning of the allowed search space as part of the optimization progresses is carried out particularly effectively. The end result is the rigorous determination of the single or multiple optimal solutions of the parameter optimization, regardless of their location, their number, and the starting values of optimization.

The methods are particularly powerful if executed in interplay with genetic optimizers generating their new populations within the currently active unpruned space. Their current best guess provides rigorous upper bounds of the minima, which can then beneficially be used for better pruning. Examples of the method and its performance will be presented, including the determination of all operating points of desired tunes or chromaticities, etc. in storage ring lattices.

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1. Introduction

The Differential Algebraic method has been successful for the description of weakly nonlinear systems, and has been utilized to compute high order transfer maps of various kinds of systems in beam- and particle optics. In addition to the computation of maps, the method

also enables various algorithms to analyze such systems efficiently [1]. Its first implementation was in the code COSY INFINITY [2–4], and it is now used in a wide variety of other codes as well [5–11]. Considering the method of Differential Algebras allows the computation of Taylor expansions on computers, one of the natural extensions is to consider the errors of the expansion, which can be captured in terms of the Taylor remainder. It is possible to obtain bounds of remainder errors on computers, and the method of remainder enhanced Differential Algebras, also called the Taylor model method [12–15], has been developed as an enhancement to the framework of Differential Algebras.

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The method has broad applications, and this paper covers one of them, namely the use for rigorous global optimization. Enhanced by the remainder error bound, the method naturally allows to obtain bounds of a function of interest. The next section reviews the Taylor model method, followed by a section discussing some function range bounding schemes, leading to a realization of a rigorous global optimization algorithm. We will demonstrate the performance of the rigorous global optimization using the Taylor model method, first using small but difficult examples, and then showing practical problems that may be encountered in common computations in beam optics and in any other fields.

2. The Taylor model method

We begin with the definition of the Taylor model, which combines the Taylor expansion at a given reference point with an enclosure for the remainder error over a domain.

Definition 1 (*Taylor model*). Let $f : D \subset \mathbb{R}^v \rightarrow \mathbb{R}$ be a function that is $(n+1)$ times continuously partially differentiable on an open set containing the v -dimensional domain D . Let x_0 be a point in D and P the n -th order Taylor polynomial of f around x_0 . Let I be a bound interval such that

$$f(x) \in P(x-x_0) + I \quad \text{for all } x \in D. \quad (1)$$

Then we call the pair (P, I) an n -th order Taylor model of f around x_0 on D .

To relate to the Differential Algebraic method, the polynomial P is the n -th order Differential Algebraic vector to represent f around x_0 , and the deviation of f from P is confined between the lower and the upper bound of I over D , thus the Taylor model (P, I) forms two hypersurfaces $P+I$ that encloses f on D rigorously. We proceed to define the arithmetic in Taylor models.

Definition 2 (*Addition and multiplication*). Let $T_{1,2} = (P_{1,2}, I_{1,2})$ be n -th order Taylor models around x_0 over the domain D . We define

$$T_1 + T_2 = (P_1 + P_2, I_1 + I_2)$$

$$T_1 \cdot T_2 = (P_{1,2}, I_{1,2})$$

where $P_{1,2}$ is the part of the polynomial $P_1 \cdot P_2$ up to order n and

$$I_{1,2} = B(P_e) + B(P_1) \cdot I_2 + B(P_2) \cdot I_1 + I_1 \cdot I_2$$

where P_e is the part of the polynomial $P_1 \cdot P_2$ of orders $(n+1)$ to $2n$ and $B(P)$ denotes a bound of P on the domain D .

These operations allow the computation of Taylor models for sums and products of two functions f and g from the Taylor models of f and g [12]. With addition and multiplication defined on Taylor models, one can now also define intrinsic functions for the Taylor models by performing various manipulations. Refer to Refs. [12,13] to see how to employ manipulations for each intrinsic function to achieve computed remainder bounds of sufficient sharpness. Finally it is straightforward to obtain an integral of a Taylor model, because obtaining the integral with respect to variable x_i of P is straightforward, thus we have an antiderivation operation ∂_i^{-1} in the Taylor model arithmetic as well.

As introduced, the method has the following properties. It provides enclosures of any function given by a finite computer code list by a Taylor polynomial and a remainder bound with a sharpness that scales with order $(n+1)$ of the width of the domain. It alleviates the dependency problem in the calculation [16,17], and it scales favorable to higher dimensional problems.

A realization of Taylor models and the arithmetic has been implemented in the code COSY INFINITY [3], first released in version 8 [18], and followed by adding improvements and more advanced algorithms. The implementation is intimately tied to that of the

Differential Algebras in COSY INFINITY, hence all the advantageous features in the Differential Algebras package such as the sparsity support and the efficient coefficient addressing scheme are inherited to the Taylor model implementation [19], making it a realistic device to study practical problems as we will show in some examples. Another advantageous feature in the implementation is to have the Taylor coefficients adhere to floating point numbers. This has practical benefits starting from the smooth connection between the Differential Algebras and the Taylor models, as well as the applicability of some powerful algorithms such as Differential Algebra fixed point solvers and some others [1]. However, it requires careful handling of errors associated to floating point numbers to maintain mathematical rigor and correctness of the arguments.

As a method to obtain rigorous estimates, interval arithmetic has been known (see for example Refs. [17,20,21]). While providing rigorous estimates, the method suffers from some practical difficulties such as the dependency problem [16], leading to over estimations to the extent that the estimates may be rigorous but at times practically useless. The Taylor model implementation in COSY INFINITY has succeeded in obtaining rigorous estimates with a minor additional computational cost, based on the superb performance of the Differential Algebras in the code.

The first natural application of the Taylor model method is range bounding of a given function f over a sufficiently small domain D . In fact, if the remainder bound I of the Taylor model (P, I) over D is sharp enough, even crudely bounding P by merely evaluating it in interval arithmetic serves the purpose often [16] and others will be briefly discussed below. As a natural consequence of these bounds, it is possible to develop methods for rigorous global optimization, based on iteratively decomposing the domain of interest until sub-regions can be shown to produce function values lying above an already established upper bound of the minimum, and then discarding these regions. The availability of the antiderivation ∂_i^{-1} in the arithmetic leads to applications such as rigorous ODE solvers for the flow [22–24], to obtain transfer maps with error estimate [14,15]. Other algorithms can be realized, and for details of the method and the implementation, refer to, for example, Refs. [12,13].

3. Bounds and rigorous global optimization using Taylor models

As mentioned, the simplest method of function range bounding using the Taylor model method is to evaluate P in interval arithmetic and add the remainder bound I , and there are various methods based on this approach [12]. However, the exact definition of the Taylor models (1) suggests the immediate availability of richer information on the function f that enables more sophisticated schemes for range bounding.

The behavior of a function f is characterized primarily by the linear part, where the accuracy of the linear representation increases as the domain of interest becomes smaller, except when there is a local extremum, in which case the quadratic part becomes the leading representative of the function. Since Taylor models have linear and quadratic terms explicitly as coefficients of P , there is no need for further efforts to obtain them. This is a significant advantage of Taylor models compared to other rigorous methods like the interval method that does not have any automated mechanism to obtain such information.

The idea leads to some Taylor model-based range bounders, first utilizing the linear part, second utilizing the quadratic part [12], and even utilizing the full Taylor polynomial up to the n -th order. Among them, the Linear Dominated Bounder (LDB) [12,25,26] and the Quadratic Fast Bounder (QFB) [25,26] are practically economical while providing excellent range bounds [13,25,26]. Both bounders are

implemented to work for multi-dimensional cases, and both can be used for multi-dimensional pruning to eliminate the area in the domain which does not contribute to range bounding. For LDB, the result of pruning can be fed back to re-evaluate the linear part in the remaining domain, resulting in the iterative refinement of bounds. Furthermore, the low end point in the domain can be used to provide a cutoff value for pruning, allowing for the scheme obtaining ultimately accurate bound if the function is monotonic.

As for the Quadratic Dominated Bounder (QDB) [12], it is difficult to implement an economical general tool for multi-dimensional cases, because a ν -dimensional quadratic range bounding problem produces cascading lower dimensional quadratic bounding problems on all the lower dimensional boundary surfaces unless the quadratic part is positive definite. This, on the other hand, leads to a special purpose quadratic bounder limiting to only positive definite cases, the Quadratic Fast Bounder (QFB). In particular it is advantageous in the situation when LDB does not work well in a local domain due to proximity to an isolated interior minimizer, which is the case when the local quadratic part of the function is positive definite. Thus LDB and QFB complement each other very well.

When those efficient tools for range bounding are used, it can lead to an efficient rigorous global optimization tool for general purpose. The key to the success is to combine all the economically available information of the objective function and the resulting tools in a smart way. For a given multi-dimensional box representing part of the search domain, we apply a branch-and-bound approach that proceeds as follows. Bound the function from below over the box, and if the lower bound is above the cutoff value, the box is eliminated from the task. Here the bounding tools are to be used in a hierarchical way, and even when the box cannot be eliminated, pruning of the box may happen when LDB or QFB is applied. If the box is not eliminated, bisect it to keep in the task unless the box size falls below the pre-specified discretization limit. The cutoff value is to be updated as efficiently as possible. When working on a box, the function value at the center point of the box, which is easy to obtain, can be used for a possible update of the cutoff value. Any other point in the search domain can be used to provide a possible update of the cutoff value. For example, some information obtained while using QFB might bring a good candidate point, and any other way is beneficial as long as it is economical. The branch-and-bound method is easily adjustable to parallel computing environment, then more sophisticated non-rigorous schemes such as global genetic optimization algorithms can be used complementarily to obtain better cutoff values globally.

For the more detailed description of the schemes, refer to Refs. [12,25,26].

4. Illustrative benchmark challenges for rigorous global optimization

4.1. A sharp isolated local minimum

To illustrate the performance of the discussed method of rigorous global optimization, we use a well known, difficult two-dimensional test problem. We ask to find the minimum and the minimizer of the function

$$f(x,y) = \cos x \cos y - 2 \exp[-500 \cdot ((x-1)^2 + (y-1)^2)]. \tag{2}$$

The first term represents the majority of the behavior of the function with the value varying periodically between -1 and 1 . On the other hand, the second term represents an extremely sharp negative spike localized around $(1,1)$, which in fact contains the actual minimum of the function. Fig. 1 shows the profile of the function with the negative spike visible, where it should be noted that the picture required a careful selection of setting such as the line sampling spacing, and the spike could be completely missed if it is drawn casually. For similar reasons, most conventional optimization methods without rigorous estimates miss the spike as will be shown below.

The code COSY INFINITY [3] has three non-rigorous optimizers, the Simplex method, the LMDIF program based on an improved Levenberg–Marquardt algorithm, and the Simulated Annealing method, thus covering different groups of typical non-rigorous optimization methods. For a given problem, besides setting up a good objective function that depends on the parameters to be optimized, the user has to choose a suitable method and assign good starting values for the parameters.

We chose the starting parameter values $(-0.1, -0.1)$ purposely to confuse the optimizers a little instead of giving more naive starting values like $(0,0)$. The processes of the optimization tasks are schematically shown by marking the parameter values at each optimization step in Fig. 1. Also marked is the true minimizer that is obtained using the rigorous global optimization. The result is summarized in Table 1,

Table 1
The minimum search of the function (2).

Algorithm	Guarantee	Steps	Min
Simulated Annealing	No	1000	~ -1
Simplex	No	130	~ -1
LMDIF	No	27	~ 0
COSY-GO, IN ⁽¹⁾	Yes	161	1.7^{08}_{16}
COSY-GO, IN ⁽²⁾	Yes	7699	1.70817^{67}_{85}
COSY-GO, TM	Yes	129	$1.7081767521607^{26}_{39}$

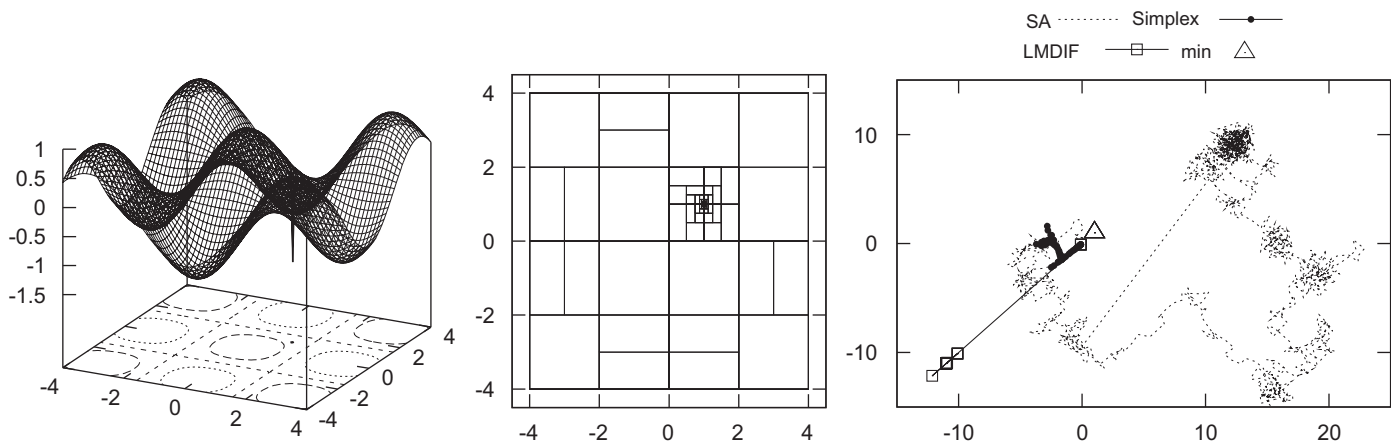


Fig. 1. The minimum search of the function (2). (Left) Profile of the function. (Middle) Branch-and-bound using the Taylor model method. (Right) Non-rigorous search by Simulated Annealing, Simplex, and LMDIF methods.

and the outcome varies wildly depending on the starting parameter values, with the best performing optimizer altering accordingly.

The Simulated Annealing method moves around like a random walk while stochastically trying neighboring values, hence it does not produce a completely wrong result, but it cannot reach to a highly accurate result after many steps; the best accuracy obtained by changing the starting values was around 10^{-2} . The performance of LMDIF fluctuates wildly depending on the situation. For instance, the starting parameter values (0,0) yield to reach the minimum with accuracy 10^{-10} in about 35 steps. When the starting values are just slightly different, it will be trapped at a wrong local extremum. The example case is that the preceding direction encounters a local saddle point, letting the optimizer misinterpret it as a local minimum and being trapped there. The Simplex method may be the most robust optimizer among three, as it performs well overall without producing a completely wrong result, though it does not help much for this example problem.

Shown also in Fig. 1 and Table 1 are the situation of heuristic and rigorous global optimizations. The domain $[-4,4]^2$ is searched for the guaranteed global minimum using the branch-and-bound method implemented in the Taylor model-based optimizer COSY-GO. We compared two approaches, the Taylor model method utilizing the advantageous features as discussed in the previous section, and the interval method representing conventional rigorous numerical methods.

The Taylor model-based COSY-GO reaches the true minimum with 10^{-14} accuracy in 129 steps at the minimizer localized within a volume 5×10^{-17} . The minimum and the minimizer are found bounded sharply as

$$\min = -1.7081767521607_{39}^{26} \quad \text{at } x = y = 1.0002272_{85}^{92}.$$

It is worth noting that the minimizer is not located exactly at (1,1), but it is slightly shifted towards the down-hill direction of the neighboring periodic hills. Fig. 1 shows each box at the time it is eliminated from consideration in the branch-and-bound approach, clearly revealing the process of branching into smaller boxes near the area of relevance. Indeed, the area containing the true minimizer can be recognized by many branched boxes gathered. In this example, there is only one such area observed. For more complicated problems, one observes multiple areas having many branched boxes gathered, due to multiple minimizers and local minima whose values are close to the true minimum, as seen in Fig. 3. Even in Fig. 1, apart from the true minimizer area, one can observe more branched boxes in the low basin areas than the hill top areas.

When the branch-and-bound method is applied based only on the interval method, the achievable accuracy becomes quite low. Table 1 lists two such cases under different accuracy demands. The first case (1) reaches a solution in 161 steps with quite low accuracy and the achieved minimizer localization volume is 2.5×10^{-4} . The second case (2) reaches a solution with moderately high accuracy

with the minimizer localized in the volume 6×10^{-9} , but the task required 7699 steps, and an attempt to achieve yet higher accuracy becomes impractical.

4.2. Other complicated challenges

In addition to the small illustrative problem discussed above, there is a large number of other known optimization challenges, each of which representing a particular trap to try to fool optimization tools. As an example, the Rosenbrock function is a typical text book optimization problem, particularly known to be difficult for gradient based methods. The Beale function is difficult for rigorous optimization methods due to a wide shallow basin which suffers from the so-called “cluster effect”. Moore’s one-dimensional polynomial problem is a milestone problem for practical rigorous optimization methods due to the “cancellation problem” which triggers the cluster effect. For more detail on the performance of the Taylor model method on these problems, the reader is referred to Refs. [25,26].

5. Design parameter search: stability regions of accelerator lattices

We now apply the rigorous global optimization method to analyze a realistic challenging problem in beam optics, the properties of a triple bend achromat (TBA) structure in the Advanced Light Source (ALS) at Lawrence Berkeley National Laboratory by studying a wide range of strength of three quadrupole magnets, k_{QF} , k_{QD} and k_{QFA} [27]. The linear lattice description of the TBA and the linear transfer map depending on k_{QF} , k_{QD} and k_{QFA} were provided by Wan at LBNL [28]. The challenge was to analyze the design parameter settings globally to meet certain properties such as a stable operation regions and desired tunes, and find all possible operating solutions for further analysis. The very first attempt, in general, would be to scan the entire range of parameter space. Work based on this approach was reported in Ref. [27]. While the approach is simple and easy to conduct technically, in practice, the fine-ness of the discretization coupled with dimensionality of the problem leads to excessively challenging computational problems. For the purpose of comparison, the non-rigorous method developed in Ref. [27] requires a computation cost that is about 1000 times larger than the fully rigorous analysis with the COSY-GO rigorous global optimizer, which we discuss now.

Specifically, we study the stable operation regions of the TBA system by scanning and by the Taylor model-based rigorous global optimization method over the parameter space domain

$$(k_{QF}, k_{QD}, k_{QFA}) \in [-10, 10]^3.$$

For the purpose of illustration and comparison with our rigorous tools, we first scan the entire domain with a discretization size

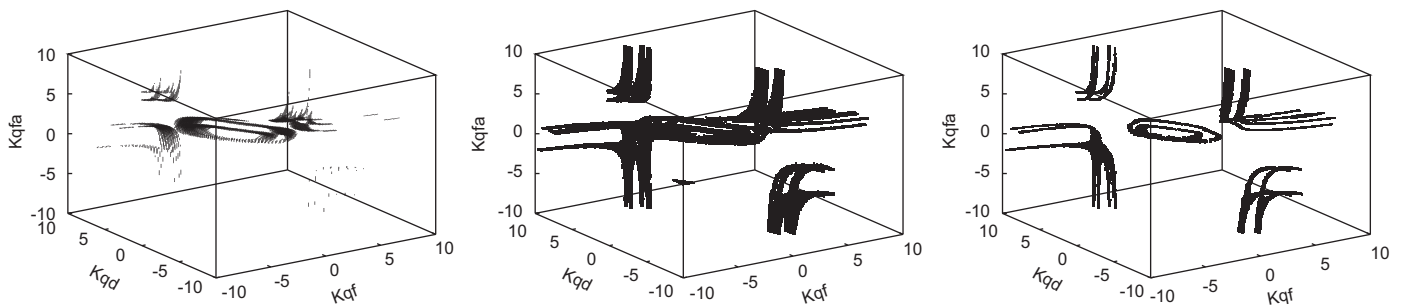


Fig. 2. Analysis of the ALS-TBA. The stable region search by scanning (left), and by the Taylor model-based rigorous global optimization (middle). The tune fitting by the Taylor model-based rigorous global optimization (right).

0.1 in each parameter, thus consisting of $201 \times 201 \times 201 \approx 8.12 \times 10^6$ scanning points. At each scanning point, the x and y trace tr_x and tr_y are computed, and only those points satisfying

$$|\text{tr}_x| < 2, \quad |\text{tr}_y| < 2 \quad (3)$$

are retained; they are shown in the left picture in Fig. 2. An equivalent computation was conducted by COSY-GO using the Taylor model method, and the obtained parameter regions are shown in the middle picture.

As the default scope of COSY-GO is to search globally the minimum of a multivariate function and the minimizer(s) rigorously, the condition (3) is altered to an optimization problem to search the minimum of the following function. Since one of the advantageous features of the Taylor model method is bounding a multivariate function sharply, the condition (3) fits naturally to the Taylor model method. However, for conducting the task here, we just limited ourselves to use only the default scope of COSY-GO:

$$f(k_{QF}, k_{QD}, k_{QFA}) = (\text{tr}_x^2 - 1.9^2)^2 + (\text{tr}_y^2 - 1.9^2)^2. \quad (4)$$

If there exist parameter values in the search domain to yield 0 to the function (4), they provide a stable operation region. Using COSY-GO, indeed the minimum of the objective function (4) was found to be 0, and the parameter regions for the minimizers are shown in the middle picture in Fig. 2. It can be seen that the rigorous optimizer indeed properly classifies the regions of relevance, but does so at a computational cost about 1000 times lower than the scanning in Ref. [27].

Next we ask to search the parameter regions yielding pre-specified tunes, as an example

$$v_x = 0.63, \quad v_y = 0.53.$$

We run COSY-GO for the following objective function:

$$f(k_{QF}, k_{QD}, k_{QFA}) = (\text{tr}_x^2 - [\text{tr}_x(v_x = 0.63)]^2)^2 + (\text{tr}_y^2 - [\text{tr}_y(v_y = 0.53)]^2)^2. \quad (5)$$

It turned out that the TBA system has quite a big range of the parameter regions yielding the desired tunes as shown in the right picture in Fig. 2. However, to conduct the same tune fitting task by scanning is very difficult if not impossible. For example, among all the stable points found by scanning as shown in the left picture, the data is processed to find the closest parameter values near the desired tunes, and they are $(k_{QF}, k_{QD}, k_{QFA}) = (1.7, -1.1, 1.4)$, with the tune values $v_x = 0.6292, v_y = 0.5417$.

To illustrate the processes of the rigorous global optimization method, the tune fitting problem is brought to a two-dimensional problem by fixing the value of k_{QFA} :

$$(k_{QF}, k_{QD}) \in [-10, 10]^2, \quad k_{QFA} = 0.$$

The boxes produced by the branch-and-bound method are recorded in Fig. 3 in the same manner as in Fig. 1. There are six optimal parameter regions found, which enclose the parameter values yielding the desired tune values exactly. Starting from the entire domain $[-10, 10]^2$ at the top, the pictures are zoomed into an interesting area near $(k_{QF}, k_{QD}) = (-3.8, 7)$ toward the bottom. The demanded box branching limit size here is 0.01. Two different methods are used for a comparison. The left pictures show the case utilizing the Taylor model method, and the right pictures with the interval method. The Taylor model method narrowed down the volume of the solution regions very sharply to 2×10^{-4} in 1370 steps, on the other hand the interval method achieved the volume to 8×10^{-3} in 2718 steps, as one can observe the performance difference merely from the pictures. Almost the same computational time was spent by both cases. While the top pictures covering the entire domain look similar between the two methods, the zoomed in pictures look quite different. The irregularly branched boxes observed in the Taylor model method case are the result of pruning by the LDB bounding method, and some cases

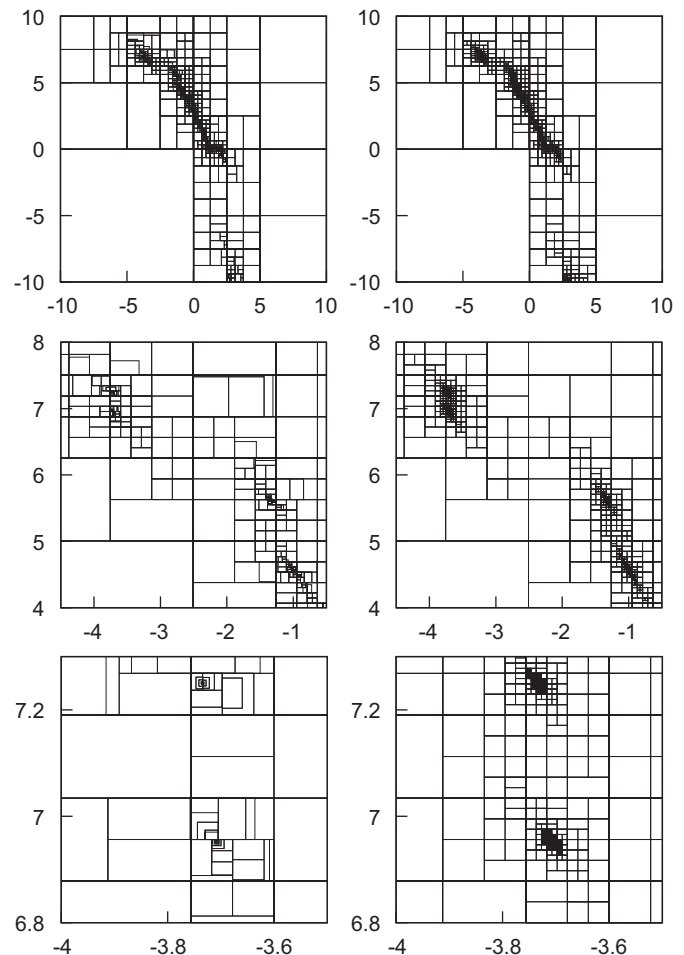


Fig. 3. Illustration of branch-and-bound to find optimal regions satisfying a given condition (left) using the Taylor model method, and (right) using the interval method, zooming into an interesting region from top to bottom. The optimal regions are painted solid black.

are due to the pruning by the QFB bounding method, which appears characteristically with three or four side pruning, and one sees such examples near $(k_{QF}, k_{QD}) = (-3.7, 7.25)$. Another aspect is that the Taylor model method provides sharper bounds without needing to branch further, and it is observed near $(k_{QF}, k_{QD}) = (-3.8, 7.1)$.

Because of limitations of space, we restrict our study of practical beam physics problems to the one above; but we hope that the example can convey the usefulness for the method for other problems as well.

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