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## Upper Bounding in Inner Regions for Global Optimization under Inequality Constraints

Ignacio Araya · Gilles Trombettoni ·  
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**Abstract** In deterministic continuous constrained global optimization, upper bounding the objective function generally resorts to local minimization at several nodes/iterations of the branch and bound. We propose in this paper an alternative approach when the constraints are inequalities and the feasible space has a non-null volume. First, we extract an *inner region*, i.e., an entirely feasible convex polyhedron or box in which all points satisfy the constraints. Second, we select a point inside the extracted inner region and update the upper bound with its cost. We describe in this paper two original inner region extraction algorithms implemented in our interval B&B called *IbexOpt* [27]. They apply to nonconvex constraints involving mathematical operators like  $+$ ,  $\cdot$ ,  $/$ , *power*, *sqrt*, *exp*, *log*, *sin*. This upper bounding shows very good performance obtained on medium-sized systems proposed in the COCONUT suite.

**Keywords** Global optimization · Upper bounding · Intervals · Branch and bound · Inner regions · Interval Taylor

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## 1 Introduction

In deterministic constrained global optimization, upper bounding the objective function consists in finding a feasible point that improves the best cost already found in the branch and bound. Most global optimizers resort to local minimization<sup>1</sup> using a Lagrangian relaxation. The considered function is sometimes big, which may render the local minimization slow.

This paper describes an alternative approach for constrained global optimization. This approach avoids the cost of evaluating the objective function repeatedly. It however requires the feasible space formed by the *inequality* constraints to have a non-null volume. More precisely, the continuous global optimization problem we handle is defined by:

$$\min_{x \in [x]} f(x) \text{ subject to } g(x) \leq 0,$$

where  $f : \mathbb{R}^n \rightarrow \mathbb{R}$  is the real-valued objective function and  $g : \mathbb{R}^n \rightarrow \mathbb{R}^m$  is a vector-valued function.  $x = (x_1, \dots, x_i, \dots, x_n)$  is a vector of variables varying in a box  $[x]$ .<sup>2</sup>  $x$  is said to be *feasible* if it satisfies the constraints.

The main idea is to exploit so-called *inner regions*, i.e., subsets of the search space in which all points are feasible.

Two communities working on interval methods have proposed several heuristics for checking whether a given domain is an inner box or, more interestingly, extracting inner boxes inside a given domain (outer box). The interval (numerical) analysis community has especially studied linear systems with interval coefficients [24, 25]. The constraint programming community has proposed general-purpose heuristics for non convex systems of inequality constraints [9, 4, 10].

Two original inner region extraction algorithms are described in this paper. These heuristics are applied for the first time to general-purpose constrained global optimization. At every node (iteration) of our interval B&B named **IbexOpt** [27], the cost is bounded above by using two inner region extraction heuristics called **InnerPolytope** and **InHC4**.

The **InnerPolytope** algorithm, described in Section 3, builds a hyperplane for every inequality constraint. The hyperplane is produced by a special convex form of interval Taylor where the expansion point is chosen at a corner of the studied outer box. If it succeeds in building an inner polytope, the point minimizing an over-estimated linearized form of the objective function is used to update the upper bound.

**InHC4** is a completely different approach that makes no linearization. On the other hand, the inner region has a more basic shape, namely a box. It is based on an operator-wise decomposition of each function and is described in Section 4. It first tries to extract an inner box from the current outer box constraint per constraint. If it fails, it simply picks a point randomly inside

<sup>1</sup> We consider minimization in this paper without loss of generality.

<sup>2</sup> An interval  $[x_i] = [\underline{x}_i, \overline{x}_i]$  defines the set of reals  $x_i$  s.t.  $\underline{x}_i \leq x_i \leq \overline{x}_i$ . A *box*  $[x]$  is the Cartesian product of intervals  $[x_1] \times \dots \times [x_i] \times \dots \times [x_n]$ .

the outer box and checks its feasibility. If it succeeds, a simple monotonicity analysis of  $f$  replaces the intervals of the monotonic variables by the adequate bounds in the found inner box and the other values are randomly chosen (no additional feasibility check is necessary since all the points in the box returned by **InHC4** are feasible). The feasible point thus obtained is used to update the upper bound.

Contrary to existing approaches, the proposed inner region extraction algorithms separate the feasibility part (handled first, by inner region extraction) and the computation of the cost (handled next, inside the found inner region).

Section 5 highlights that, like the other inner region extraction algorithms, our algorithms are heuristics. In other words, they sometimes fail to find an inner region even if one such region exists. However, the same section underlines that they are rather inexpensive.

The experiments shown in Section 6 highlight that this upper bounding policy, with the two procedures **InnerPolytope** and **InHC4**, brings very good speedups to our interval B&B **IbexOpt** [27].

## 2 Background and handled problem

Intervals allow reliable computations on computers by managing floating-point bounds and outward rounding.

### Intervals

An **interval**  $[x_i] = [\underline{x}_i, \overline{x}_i]$  defines the set of reals  $x_i$  s.t.  $\underline{x}_i \leq x_i \leq \overline{x}_i$ , where  $\underline{x}_i$  and  $\overline{x}_i$  are floating-point numbers.  $\mathbb{IR}$  denotes the set of all intervals. The size or **width** of  $[x_i]$  is  $w([x_i]) = \overline{x}_i - \underline{x}_i$ . A **box**  $[x]$  is the Cartesian product of intervals  $[x_1] \times \dots \times [x_i] \times \dots \times [x_n]$ . Its width is defined by  $\max_i w([x_i])$ .  $m([x])$  denotes the middle of  $[x]$ . The **hull** of a subset  $S$  of  $\mathbb{R}^n$  is the smallest  $n$ -dimensional box enclosing  $S$ .

*Interval arithmetic* [20] has been defined to extend to  $\mathbb{IR}$  elementary functions over  $\mathbb{R}$ . For instance, the interval sum is defined by  $[x_1] + [x_2] = [\underline{x}_1 + \underline{x}_2, \overline{x}_1 + \overline{x}_2]$ . When a function  $f$  is a composition of elementary functions, an *extension* of  $f$  to intervals must be defined to ensure a conservative image computation.

### Definition 1 (Extension of a function to $\mathbb{IR}$ ; inclusion function; range enclosure)

Consider a function  $f : \mathbb{R}^n \rightarrow \mathbb{R}$ .

$[f] : \mathbb{IR}^n \rightarrow \mathbb{IR}$  is said to be an **extension** of  $f$  to intervals iff:

$$\begin{aligned} \forall [x] \in \mathbb{IR}^n \quad [f]([x]) &\supseteq \{f(x), x \in [x]\} \\ \forall x \in \mathbb{R}^n \quad f(x) &= [f]([x, x]) \end{aligned}$$

The **natural extension**  $[f]_N$  of a real function  $f$  corresponds to the mapping of  $f$  to intervals using interval arithmetic. The inner interval linearizations proposed in this paper is related to the first-order **interval Taylor extension** [20], defined as follows:

$$[f]_T([x]) = f(\tilde{x}) + \sum_i [a_i] \cdot ([x_i] - \tilde{x}_i)$$

where  $\tilde{x}$  denotes any point in  $[x]$ , e.g.,  $m([x])$ , and  $[a_i]$  denotes  $\left[ \frac{\partial f}{\partial x_i} \right]_N([x])$ .

Equivalently, we have:  $\forall x \in [x], \underline{[f]_T([x])} \leq f(x) \leq \overline{[f]_T([x])}$ .

*Example.* Consider  $f(x_1, x_2) = 3x_1^2 + x_2^2 + x_1x_2$  in the box  $[x] = [-1, 3] \times [-1, 5]$ . The natural evaluation provides:  $[f]_N([x_1], [x_2]) = 3[-1, 3]^2 + [-1, 5]^2 + [-1, 3][-1, 5] = [0, 27] + [0, 25] + [-5, 15] = [-5, 67]$ . The partial derivatives are:  $\frac{\partial f}{\partial x_1}(x_1, x_2) = 6x_1 + x_2$ ,  $\left[ \frac{\partial f}{\partial x_1} \right]_N([-1, 3], [-1, 5]) = [-7, 23]$ ,  $\frac{\partial f}{\partial x_2}(x_1, x_2) = x_1 + 2x_2$ ,  $\left[ \frac{\partial f}{\partial x_2} \right]_N([x_1], [x_2]) = [-3, 13]$ . The interval Taylor evaluation with  $\tilde{x} = m([x]) = (1, 2)$  yields:  $[f]_T([x_1], [x_2]) = 9 + [-7, 23][-2, 2] + [-3, 13][-3, 3] = [-76, 94]$ .

Handled problem

A continuous constrained global optimization problem is defined as follows.

**Definition 2 (Constrained global optimization)**

Consider a vector of variables  $x = (x_1, \dots, x_i, \dots, x_n)$  varying in a box  $[x]$ , a real-valued function  $f : \mathbb{R}^n \rightarrow \mathbb{R}$ , vector-valued functions  $g : \mathbb{R}^n \rightarrow \mathbb{R}^m$  and  $h : \mathbb{R}^n \rightarrow \mathbb{R}^p$ .

Given the system  $S = (f, g, h, [x])$ , the constrained global optimization problem consists in finding:

$$\min_{x \in [x]} f(x) \quad \text{subject to} \quad g(x) \leq 0 \wedge h(x) = 0.$$

$f$  denotes the **objective function**;  $g$  and  $h$  are **inequality and equality constraints** respectively.  $x$  is said to be **feasible** if it satisfies the constraints.

Our interval optimizer extracts *inner boxes* and *inner polytopes* inside classical (outer) boxes.

**Definition 3** Consider a system  $(f, g, [x])$  comprising only inequality constraints. An **inner region**  $r^{in}$  is a feasible subset of  $[x]$ , i.e.,  $r^{in} \subset [x]$  and all points  $x \in r^{in}$  satisfy  $g(x) \leq 0$ .

Only a few softwares rigorously solve the constrained global optimization defined above. Several global optimizers based on an interval B&B, like GlobSol [12] and Icos [14], return a tiny box guaranteed to contain a real-valued vector  $x$   $\epsilon$ -minimizing:  $f(x)$  s.t.  $g(x) \leq 0 \wedge h(x) = 0$ .<sup>3</sup>

<sup>3</sup>  $\epsilon$ -minimize  $f(x)$  means minimize  $f(x)$  with a precision  $\epsilon$ , i.e., we have  $f(y) \geq f(x) - \epsilon$ , for all (feasible)  $y$ .

Inspired by the IBBA solver [22], we propose to relax pure equalities  $h_j(x) = 0$  by “thick” equations  $h_j(x) \in [-\epsilon_{eq}, +\epsilon_{eq}]$ , i.e., two inequalities:  $-\epsilon_{eq} \leq h_j(x) \leq +\epsilon_{eq}$ . Therefore, our `IbexOpt` global optimizer [27] rigorously computes a floating-point vector  $x$   $\epsilon$ -minimizing:

$$f(x) \text{ s.t. } g(x) \leq 0 \wedge (-\epsilon_{eq} \leq h(x) \leq +\epsilon_{eq}).$$

Note that IBBA and `IbexOpt` can only guarantee the global optimum of the relaxed system, although  $\epsilon_{eq}$  can often be chosen almost arbitrarily small. Also note that most of the deterministic global optimizers (generally based on a spatial branch and bound), like Baron [26] or Couenne [3], can guarantee the solution neither to the constrained global optimization problem (Definition 2) nor to the relaxed problem. Finally note that, in practice, most of the equations are already “thick” and thus do not need to be further relaxed with an  $\epsilon_{eq}$ . Equations modeling physical systems often have indeed at least one coefficient that can be represented by an interval constant. This parameter corresponds to a bounded uncertainty, e.g., an imprecision on a measurement.

In the sake of simplicity, since our optimizer accepts inequalities and relaxed equalities that are also inequalities, we consider from now on that the handled constrained global optimization problem is:

$$\min_{x \in [x]} f(x) \text{ s.t. } g(x) \leq 0,$$

i.e., the functions  $h(x) - \epsilon_{eq}(\leq 0)$  and  $-h(x) - \epsilon_{eq}(\leq 0)$  belong to the vector  $g : \mathbb{R}^n \rightarrow \mathbb{R}^m$  of functions.

Note that numerous convex and nonconvex mathematical operators can be taken into account, such as  $+$ ,  $\cdot$ ,  $/$ ,  $x^n$ ,  $exp$ ,  $log$ ,  $sqrt$ ,  $sine$ , etc.

### 3 Inner polytope algorithm

The main idea is to build a half-space for each inequality  $g_j(x) \leq 0$ , such that *all* the points in the computed half-space satisfy the constraint. For that purpose, we use a specific first order interval Taylor form of a nonlinear function. The usual first-order interval Taylor form, defined in Section 2, can select any expansion point  $\tilde{x}$  inside the box to achieve the linearization. Instead of the usual midpoint, a *corner* of the box is chosen here, i.e.,  $\underline{x}$ .

Consider a function  $g_j : \mathbb{R}^n \rightarrow \mathbb{R}$  and a domain  $[x]$ . For any variable  $x_i \in x$ , let  $[a_i^j]$  be  $\left[ \frac{\partial g_j}{\partial x_i} \right]_N([x])$ . The idea is to bound  $g_j(x)$  from above with an affine function  $g_j^l(x)$  obtained by a corner-based interval Taylor form. For all real vector  $x \in [x]$ , we have:

$$g_j(x) \leq g_j^l(x) = g_j(\underline{x}) + \sum_i \overline{a_i^j} \cdot (x_i - \underline{x}_i). \quad (1)$$

If we consider an inequality  $g_j(x) \leq 0$ , relation (1) enables us to build a hyper-plane  $g_j^l(x) = 0$  bounding the solution/feasible set from above:  $g_j(x) \leq$

$g_j^l(x) \leq 0$ . That is to say, the linear function  $g_j^l(x)$  can be used to define an inner region of  $[x]$ .

**Proposition 1** *The interval linear form (1) is correct and rigorous, i.e., it can be made robust to computation errors over floating-point numbers.*

Rigor is ensured by the *interval* Taylor [21]. The correction of relation (1) lies on the fact that any “variable”  $(x_i - \underline{x}_i)$  is positive since its domain is  $[0, d_i]$ , with  $d_i = w([x_i]) = \overline{x}_i - \underline{x}_i$ . Therefore, maximizing each term  $[a_i^j] \cdot (x_i - \underline{x}_i)$  for any point  $(x_i - \underline{x}_i) \in [0, d_i]$  is obtained with  $\overline{a_i^j}$ .

Example

Consider the constraint

$$g_1(x_1, x_2) = x_1^3 + \cos(x_1) - \sin(x_2) - 0.15 \leq 0$$

in a box  $[x_1] \times [x_2] = [-0.32, 0.52] \times [0.90, 1.06]$ .

We can derive from the gradient of  $g_1$ :

$$\begin{aligned} - \left[ \frac{\partial g_1}{\partial x_1} \right]_N &= 3 \cdot [-0.32, 0.52]^2 - \sin([-0.32, 0.52]) = 3[0, 0.2704] - [-0.314, 0.497] \\ &= [-0.497, 1.1252] \\ - \left[ \frac{\partial g_1}{\partial x_2} \right]_N &= -\cos([0.90, 1.06]) = [-0.6216, -0.488872082] \end{aligned}$$

The function  $g_1$  is illustrated in Fig. 1. The feasible space appears in grey. Applying (1) to  $g_1$  provides:

$$g_1(-0.32, 0.90) + 1.1252(x_1 + 0.32) + -0.4889(x_2 - 0.90) \leq 0.$$

The left part of the figure shows in dark grey the corresponding inner region, a polytope obtained by intersecting this half-space with the box.

The right side of the figure shows an inner space computed by a standard interval Taylor with an expansion point taken in the middle of the box:

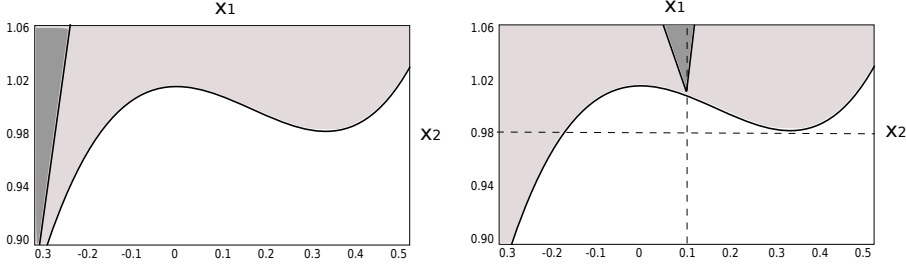
$$g_1(0.10, 0.98) + [-0.497, 1.1252](x_1 - 0.10) + [-0.6216, -0.4889](x_2 - 0.98)$$

This form implies a (non necessarily convex) union of four polytopes, each polytope being obtained by the intersection of 5 half-spaces: the first two correspond to the sign constraints (a shifted orthant, separated by dotted lines on the figure), the next two correspond to the box boundaries and the last to the Taylor expansion. For instance, the first polyhedron is:

$$\begin{cases} x_1 < m[x_1] \\ x_2 < m[x_2] \\ x_1 \geq \underline{x}_1 \\ x_2 \geq \underline{x}_2 \\ 0.0155067948 - 0.497(x_1 - 0.10) - 0.6216(x_2 - 0.98) \leq 0 \end{cases}$$

Note that two of the polytopes are empty on this example (including the one detailed above). The other two appear on the figure and are generated by the following Taylor forms:

1.  $0.0155067948 - 0.497(x_1 - 0.10) - 0.4889(x_2 - 0.98) \leq 0$  ( $x_1 < m[x_1]$  and  $x_2 > m[x_2]$ )
2.  $0.0155067948 + 1.1252(x_1 - 0.10) - 0.4889(x_2 - 0.98) \leq 0$  ( $x_1 > m[x_1]$  and  $x_2 > m[x_2]$ )



**Fig. 1 Left:** Inner polytope generated by a corner-based interval Taylor in  $(\underline{x}_1, \underline{x}_2)$ . **Right:** Two inner polytopes generated by a midpoint interval Taylor in two of the four orthants.

A linear program for a better feasible point (upper bound)

Applying this idea to the objective function  $f(x)$  and to the inequalities  $g_j(x) \leq 0$ , we can derive the linear program  $LP^{ub}$ :

$$\begin{aligned}
 LP^{ub} = \min \quad & f(\underline{x}) + \sum_i \bar{a}_i * (x_i - \underline{x}_i) \\
 \text{subject to: } \quad & \forall j \quad g_j(\underline{x}) + \sum_i \bar{a}_i^j * (x_i - \underline{x}_i) \leq 0 \\
 & \forall i \quad \underline{x}_i \leq x_i \wedge x_i \leq \bar{x}_i
 \end{aligned}$$

A Simplex algorithm solves  $LP^{ub}$  and returns infeasibility or the optimal solution  $x^l$  (see Algorithm 1). Infeasibility proves nothing because the linearized system is more constrained than the original system, so that one could still find solutions in the original one. If the Simplex algorithm returns an optimal solution of the inner approximation, then  $x^l$  is also a solution to the original system, maybe not the optimal one. The previous process is correct on

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**Algorithm 1** InnerPolytopeUB (**in:**  $S, [x]^{out}$ ; **in-out:**  $ub, x_{ub}$ )

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```

 $LP^{ub} \leftarrow \text{InnerLinearization}(S, [x]^{out})$ 
 $x^l \leftarrow \text{Simplex}(LP^{ub})$ 
if  $x^l \neq \perp$  and  $\text{FeasibilityCheck}(x^l, S)$  then
   $cost \leftarrow [f]_N([x^l, x^l])$ 
  if  $cost < ub$  then  $ub \leftarrow cost; x_{ub} \leftarrow x^l$  end if
end if

```

---



the real numbers, but is not necessarily always correct on a computer due to roundoff errors on floating-point numbers. Indeed, since we use a standard Simplex algorithm working with floating-point numbers, it is possible that the best (floating) value returned by the LP solver falls slightly outside the inner polytope and is not feasible. That is why we render the whole process rigorous by checking the feasibility of  $x$  with an interval evaluation (see line 3 of Algorithm 1).

The pseudocode finally details that one evaluates the objective function (the original one, not the linearized one) at the point  $x^l$  and potentially improves the upper bound. In this case, we update the point  $x_{ub}$  and its cost (i.e., the new upper bound)  $ub$ .

#### Related work, discussion

Interval Taylor forms have often been used to produce an *outer* linear approximation of the solution set or of the objective function. However, when the expansion point is chosen strictly inside the domain, the system obtained by an interval Taylor form is *not* convex. It forms an intersection of non-convex sub-spaces. (Examples can be found in [21, 12, 19].) Contracting optimally a box containing this non-convex relaxation has been proven to be NP-hard [13]. This explains why the interval analysis community has worked a lot on this problem for decades [23, 11, 6].

Several researchers proposed to select as expansion point of the interval Taylor form a corner of the studied box, instead of the usual midpoint [2, 15–17, 21]. The main drawback is that it leads generally to a larger system relaxation surface. The main virtue is that the approximated solution set belongs to a unique orthant and is convex, i.e., it is a polytope.

The dual form defined by (1) has never been used before to achieve an *inner* polytope extraction, and so has never been used before to improve an upper bound in constrained global optimization.

## 4 The InHC4 algorithm

InHC4 is similar to the state-of-the-art constraint propagation algorithm HC4 [4, 9, 18] to the extent that its core procedure called **InHC4-Revise** (in short **InHC4R**) is based on a forward-backward traversal of the tree representation of constraints (see Fig. 2). Furthermore, the forward phase is exactly the same as in the core procedure of HC4, called **HC4-Revise** (in short **HC4R**). However, the main loop and the backward phase are radically different, as we detail below. In addition, they do not calculate of course the same box. Let us start with the main loop.

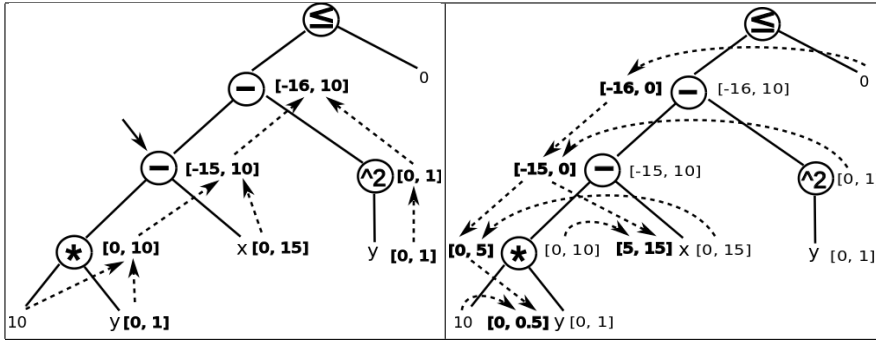
The main loop of InHC4 handles every constraint once in sequence and performs each time a call to **InHC4R**. Given an input box  $[x]$ , **InHC4R** produces an inner box  $[x]^{in} \subseteq [x]$  with respect to the constraint under process. It is

then easy to build incrementally a box that is inner with respect to the whole system. More precisely, the main loop:

- calls **InHC4R** on the  $1^{st}$  constraint with the outer box as input,
- calls **InHC4R** on the  $j^{th}$  constraint with the box obtained after the previous call (the one for the  $(j - 1)^{th}$  constraint), provided it is non empty.

Thus, if a non empty box is returned after the handling of the last constraint, then this box is inner w.r.t. all the constraints.

Let us now detail **InHC4R**. Unlike the refutation process of **HC4R**, **InHC4R** tries to extract an inner region at each operator of the constraint.



**Fig. 2** Binary tree representation of the constraint  $10y - x - y^2 \leq 0$ . **Left:** First forward evaluation phase. **Right:** backward inner projection phase.

Let us denote by  $[x]$  the input box and  $g_j(x) \leq 0$  the constraint. Each node of the tree is associated to an interval, the intervals related to the leaves are initialized with the corresponding values in  $[x]$ . Then, the following two phases are performed:

- Forward evaluation (see Fig. 2–left): The tree is traversed from the leaves to the root and intervals associated to an operator are computed with interval arithmetics. For example, the node pointed by the arrow is initialized with the interval  $[0, 10] - [0, 15] = [-15, 10]$ . Thus, every node contains an interval corresponding to the *natural* interval evaluation of the subexpression.
- Backward *inner projection* (see Fig. 2–right): From the root to the leaves, the intervals in each node are contracted using specific *inner projection* operators.

In each node related to a binary operator  $op$  and labeled with an interval  $[z]$  (i.e.,  $z = x_1 op x_2$ ), the 2-dimensional box corresponding to its children vertices  $x_1$  and  $x_2$  is reduced to an inner box  $[x_1]^{in} \times [x_2]^{in}$  such that:

$$\forall (x_1, x_2) \in [x_1]^{in} \times [x_2]^{in} : x_1 op x_2 \in [z] \quad (2)$$

If  $op$  corresponds to a unary operator (i.e.,  $z = op(x)$ ), its unique child is reduced to  $[x]^{in}$ , such that:

$$\forall x \in [x]^{in} : op(x) \in [z] \quad (3)$$

If an inner projection returns an empty box (i.e., no box satisfying (2) or (3) has been found), then the top-down process is interrupted. It means that **InHC4R** failed to find a box that is inner w.r.t.  $g_j(x) \leq 0$ . It implies that **InHC4** failed to find a box that is inner w.r.t. the  $n$  inequality constraints, so that the main loop of **InHC4** is interrupted.

Consider for instance the backward projection applied to the product operator of Fig. 2–right and its two children. The reduced intervals appear in bold in the left side of each node (e.g.,  $[z]$  is  $[0, 5]$ ). Before reduction, its children are labeled with the intervals  $[10, 10]$  and  $[0, 1]$ . They are then reduced to  $[10, 10]$  and  $[0, 0.5]$  respectively. The reduction agrees with relation (2), i.e.,  $\forall y \in [0, 0.5] : 10 \cdot y \in [0, 5]$ . The next section details how these basic inner projection operators are achieved.

#### 4.1 Inner projection for basic operators

We report in this section the main guidelines to implement the inner projection for the main mathematical operators. Four different cases must be studied and follow a monotonicity analysis. This approach extends the case-by-case approach proposed in Section 3 of [7]. We have built a more generic projection based on monotonicity properties.<sup>4</sup> The first case is trivial but serves as a basis for understanding the others.

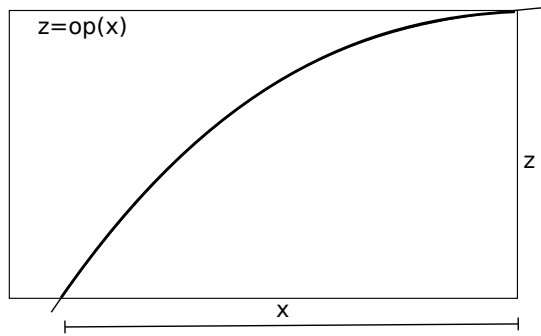
##### *Case 1: monotonic unary operators*

The first case applies to monotonic and continuous unary operators, like  $\log$  and  $\exp$ . More precisely, we consider operators  $z = op(x)$  that are continuous and monotonic w.r.t.  $x$  in  $[x]$ .

In this case, inner projection is trivial (see Fig. 3). We compute the maximum inner interval (i.e., no feasible point is lost, leaving aside roundoffs) using the inverse function of  $op$ , like in a standard projection in **HC4R**. E.g., if  $z = \exp(x)$ ,  $[x]^{in} := \log([z])$ . However, to take into account floating-point roundoff errors, the outward rounding of **HC4R** is replaced by inward rounding.<sup>5</sup>

<sup>4</sup> In addition, Chabert & Beldiceanu handled a dual problem consisting in finding a box with no solution (i.e., all points in this box violate the constraints) and required an initial point to be “inflated” to a box...

<sup>5</sup> With floating-point numbers, an interval evaluation is conservative (i.e., contains all the real-valued images) if the lower bound of the interval image is rounded towards  $-\infty$  while the upper bound is rounded to  $+\infty$ . Both rounding operations constitute a so-called outward rounding.

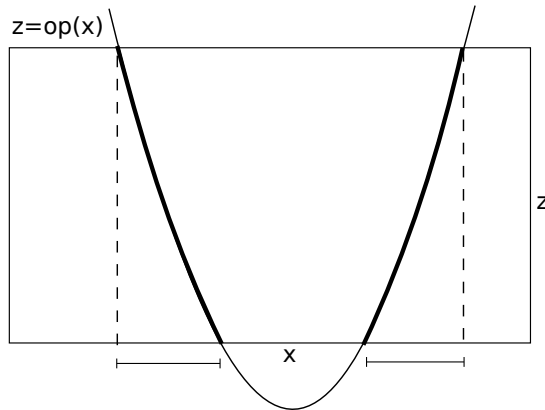


**Fig. 3** Case 1: Inner projection of a monotonic operator. The horizontal segment in the bottom of the figure is the result of the inner projection on  $x$ .

*Case 2: non monotonic unary operators*

The second case applies to non monotonic unary operators, like  $x^2$  or *sine*. More precisely, we consider operators  $z = op(x)$  that are *not* monotonic w.r.t.  $x$  in  $[x]$ .

In this case, we achieve a piecewise monotonicity analysis and obtain an interval for every monotonic part. Finally, unless the union of computed intervals forms a connected set, we select randomly one interval. Note that for



**Fig. 4** Case 2: Inner projection of a non monotonic operator, i.e., *sqr*. Two intervals (illustrated by horizontal segments) are obtained by projection on  $x$  (i.e., using the inverse operation of *sqr*), and one of them is randomly chosen and returned.

With inward rounding, the lower bound is rounded towards  $+\infty$  and the upper bound towards  $-\infty$ . The property enforced by outward (resp. inward) rounding for an operator  $op$  is (1), resp. (2):

1.  $\forall x \in [x] \exists z \in op([x]) \ z = op(x)$
2.  $\forall z \in op([x]) \exists x \in [x] \ z = op(x)$

non monotonic unary operators, the standard HC4R returns the hull of the intervals. For an inner projection in InHC4R, only a single interval is kept since holes between these intervals represent inconsistent/infeasible points (Fig. 4).

*Case 3: monotonic binary operators*

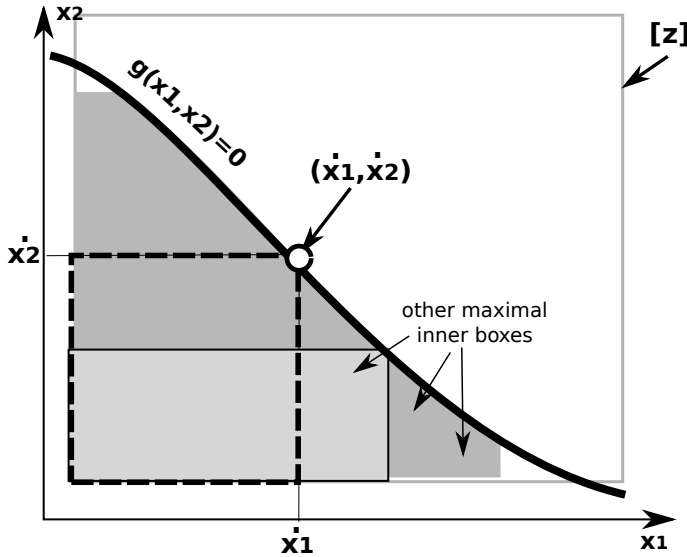
A specific handling must be carried out on *monotonic* binary operators.

**Definition 4** A function  $\mathbb{R}^2 \rightarrow \mathbb{R}$   $f(x_1, x_2)$  is *nondecreasing* (resp., *non-increasing*) *monotonic w.r.t.  $x_1$*  in  $[x_1] \times [x_2]$  if for all  $c$  in  $[x_2]$  we have:  $\forall(a, b) \in [x_1]^2, a \leq b \Rightarrow f(a, c) \leq f(b, c)$  (resp.  $a \leq b \Rightarrow f(a, c) \geq f(b, c)$ ).

$f(x_1, x_2)$  is said *monotonic* if  $f(x_1, x_2)$  is monotonic w.r.t each of its variables in  $[x_1] \times [x_2]$ .

Note that  $f$  may be for instance nondecreasing w.r.t.  $x_1$  and nonincreasing w.r.t.  $x_2$ .

For binary (or n-ary) operators that are monotonic w.r.t. each of their variables, a generic procedure, called `MonoMaxInnerBox`, can compute randomly one maximal inner box, if one such box exists, as shown in Fig. 5.



**Fig. 5** Case 3, procedure `MonoMaxInnerBox`: The dotted box corresponds to a maximal inner box of  $[z]$  w.r.t. the monotonic constraint  $g(x_1, x_2) \leq 0$ . A point  $x_1$  is randomly picked inside the range of allowed values illustrated by the horizontal segment. Only one remaining value  $x_2$  can then make the computed inner box maximal.

As depicted in Fig. 5, there usually exists an infinite number of maximal boxes so that we select randomly one of these maximal inner boxes.

Handling a monotonic binary operator amounts to handling the two inequalities

$$\underline{z} \leq (x_1 \text{ op } x_2) \leq \bar{z}.$$

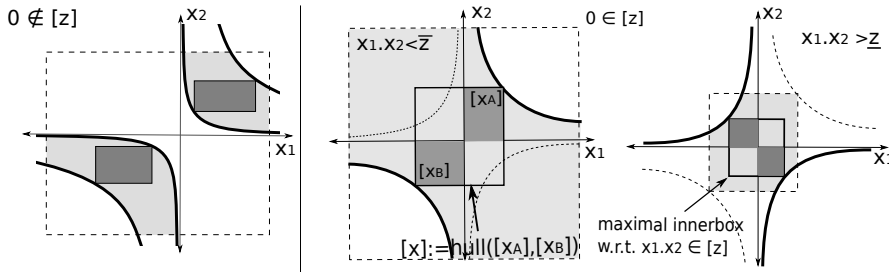
Both inequalities are handled in sequence, the inner box computed for one inequality being used as input of the second one. This procedure is of course used for implementing the inner projection of the addition and subtraction operators.

It is also used for handling several (monotonic) subcases of the non monotonic binary operators: the multiplication and the division described below.

*Case 4: non monotonic binary operators*

The last case includes the binary (or n-ary) operators that are *not* monotonic w.r.t. each of their variables, i.e., the multiplication and the division.

Fig.6 illustrates the two main cases for the multiplication  $x_1.x_2 \in [z]$ , depending whether 0 belongs or not to  $[z]$ .



**Fig. 6** Inner projection for the binary multiplication. **Left:** Two maximal boxes that can indifferently be computed by `MonoMaxInnerBox` in the two disjoint inner regions (quadrants) defined by the operator  $x_1.x_2 \in [z] \geq 0$ . **Middle and right:** Maximal box computed for  $x_1.x_2 \in [z] \ni 0$  ( $\bar{z} \geq -\underline{z}$ ) with four calls to `MonoMaxInnerBox` (boxes in grey).

For the case  $x_1.x_2 \in [z] \ni 0$ , note that a direct procedure (although more difficult to be implemented) could also be achieved without resorting to `MonoMaxInnerBox`.

Two different implementations for the division have been tested. One approach amounts to rewriting  $x_1/x_2 = x_1 \cdot \frac{1}{x_2} \in [z]$ . The other approach directly considers the different monotonic subcases of the operator, like for the multiplication. Non exhaustive experiments show that both versions seem to have the same performance in practice.

#### 4.2 Improving the upper bound using InHC4

Algorithm 2 details how `InHC4` is used by `IbexOpt` for improving the upper bound.

**Algorithm 2** Inhc4UB (**in:**  $S, [x]^{out}$ ; **in-out:**  $ub, x_{ub}$ )

---

```

 $[x]^{in} \leftarrow \text{InHC4}(S, [x]^{out})$  /* Inner box extraction */
if  $[x]^{in} \neq \emptyset$  then
   $[x]^{in} \leftarrow \text{MonotonicityAnalysis}(f, [x]^{in})$ 
   $x \leftarrow \text{RandomProbing}([x]^{in})$  // or gradient descent
else
   $x \leftarrow \text{RandomProbing}([x]^{out})$ 
end if
 $cost \leftarrow [f]_N([x, x])$  /* Cost evaluation */
if  $cost < ub$  and ( $[x]^{in} \neq \emptyset$  or  $[g]_N([x, x]) \leq 0$ ) then
   $ub \leftarrow cost$ ;  $x_{ub} \leftarrow x$ 
end if

```

---

If an inner box  $[x]^{in}$  is found by InHC4, then `MonotonicityAnalysis` analyzes the monotonicity of the objective function  $f$  w.r.t. every variable  $x_i$ . If the partial derivative  $[a_i] = \left[ \frac{\partial f}{\partial x_i} \right]_N([x]^{in}) \geq 0$ , then  $f$  is increasing w.r.t.  $x_i$  in  $[x]$ , and  $[x_i]$  is replaced by the degenerated interval  $[x_i, x_i]$  in  $[x]^{in}$  for minimizing  $f(x)$  over  $[x]^{in}$ . If  $[a_i] \leq 0$ ,  $f$  is decreasing and  $[x_i]$  is replaced by  $[\overline{x}_i, \overline{x}_i]$  in  $[x]^{in}$ .

Next, we pick randomly a point  $x$  inside the resulting box, and replace  $x_{ub}$  by  $x$  if  $x$  satisfies the constraints and improves the best cost  $ub$ . Two different cases may occur. If an inner box has been extracted by InHC4, then a point is selected inside  $[x]^{in}$ . The feasibility of  $x$  does not need to be checked since  $[x]^{in}$  contains only feasible points. If no inner box is available, a random point is still picked in the outer box  $[x]^{out}$ , and the constraints must then be checked.

Replacing this simple probing by a home-made gradient descent did not improve the strategy. However, our implementation was not sophisticated and we should try other descent algorithms (quasi-Newton, etc.) before drawing definite conclusions.

## 5 Properties

Several properties can be deduced from the material presented in the previous two sections. The first one is a negative one.

**Observation 1** *The two algorithms `InnerPolytope` and `InHC4` are correct but incomplete, i.e., they are heuristics that can sometimes miss an inner region whereas one such region does exist.*

`InnerPolytope` is incomplete because it does not calculate, in general, an inner polytope that is maximal (with respect to the inclusion), eventhough roundoff errors are left aside. The calculated polytope may be empty. This is a consequence of the overestimate produced by the interval Taylor form.

The `InHC4-Revise` procedure (handling a single constraint) is also incomplete because it overestimates the intervals in the forward phase and makes random choices in the backward phase. Indeed, if an intermediary node is

overestimated, we can choose in the backward phase a part of the domain that is not compatible with the variables. The overestimate can be induced by variables appearing several times in the function or by a discontinuity of the function. Consider for instance the constraint  $\sin(1/x) \leq 0.5$  and the domain  $[x] = [-1/\pi, 1/\pi]$ . During the forward phase, the discontinuity of  $1/x$  leads to hull  $[-\infty, -\pi] \cup [\pi, +\infty]$  to  $[-\infty, +\infty]$ . During the backward phase, choosing unluckily the monotonic part  $[-\pi/2, \pi/6]$  would lead to find no inner box.

Finally, even though **InHC4-Revise** was complete (for a single constraint), the **InHC4** algorithm could be not able to find a box that is inner to the whole system. One can observe that all the cases handled by the **InHC4R** procedure, except the first one (monotonic unary operator), ignore a part of the feasible space.<sup>6</sup> Therefore, an inner box “arbitrarily” built by **InHC4R** for a given constraint, as underlined in Section 4.1, sometimes leads to an empty inner box when handling a subsequent constraint.

The following proposition highlights an interesting aspect of **InHC4-Revise**.

**Proposition 2** *Consider a function  $g_j$  that contains at most one occurrence of each variable and is continuous in its domain  $[x]$ .*

**InHC4-Revise** *always succeeds in extracting an inner box  $[x]^{in}$  w.r.t. the constraint  $g_j(x) \leq 0$  in the domain  $[x]$ , and  $[x]^{in}$  is maximal (leaving aside roundoff errors due to floating-point arithmetic), i.e., there is no other larger box  $[x]^{in'} \supset [x]^{in}$  that is an inner box of  $[x]$  w.r.t.  $g_j$ .*

Proof (sketch)

As mentioned above, the continuity of the function  $g_j$  and the single occurrence condition are the conditions to avoid an overestimate of the basic operators during the forward phase.

We can prove that every implemented unary and binary operator computes a maximal inner box, leaving aside the loss involved by inward roundoffs. This is straightforward for cases 1 and 2. This is obtained by construction in the case 3 from the procedure **MonoMaxInnerBox**. The only difficulty lies in the proof of the case  $x_1.x_2 \in [z]$  when  $0 \in [z]$ .<sup>7</sup>

The single occurrence condition follows that of the standard **HC4R** [5]. It ensures that the expression is a tree structure and not a directed acyclic graph (because a variable appearing several times in the expression has several parents in the graph) that cannot keep the property by induction. In other terms, the condition ensures that, during the backward traversal, the composition of inner boxes provides maximal inner intervals on all the dimensions.  $\square$

<sup>6</sup> In the case 2, only one inner interval is considered among the different ones in the union. In the case 3, only one maximal inner box is computed (using a random choice on  $x_1$ ) among an infinite number of possible boxes. The last case gathers both drawbacks (from cases 2 and 3). Consider for instance the case of the multiplication  $x_1.x_2 \in [z]$  where  $z$  is positive (see left side of Fig. 6).

<sup>7</sup> The difficulty is only related to our implementation. The maximality can be more easily checked with a direct implementation.



We recall that the maximality property does not hold for a *system* of inequality constraints handled by `InHC4`. Also note that `InnerPolytope` and `InHC4` are not comparable because the box produced by `InHC4` is not necessarily included in the polytope produced by `InnerPolytope`.

A second proposition provides the worst-case time-complexity of our two inner region extraction algorithms.

**Proposition 3** *Consider a system  $(f, g, [x])$  with  $n$  variables and  $m$  inequalities. Let  $k$  be the maximum number of unary and binary operators in a function  $g_j$ . Let  $t$  the maximum time required to evaluate a primitive mathematical operator.*

*Then, the worst-time complexity of the `InnerPolytope` extraction procedure is  $O(m(k.t + n))$ . The worst-time complexity of the `InHC4` extraction procedure is  $O(m.k.t)$ .*

Proof

For `InnerPolytope`, computing a hyperplane (or generating a linearized form of the objective function) is achieved in time  $O(k.t + n)$ . Indeed, computing the gradient of a given function  $g_j$  is obtained in time  $O(k.t + n)$  with automatic differentiation; evaluating  $g_j(\underline{x})$  requires time  $O(k.t)$ ; the sum of terms  $\overline{a_i^j} \cdot (x_i - \underline{x}_i)$  is  $O(n)$  for all the variables. Finally, generating the linear program  $LP^{ub}$  amounts to  $m + 1$  calls to the previous procedure (i.e., the  $m$  constraints plus the objective function). Note that the time complexity for a call to an LP solver must be added to this time complexity in the procedure `InnerPolytopeUB`.

The procedure `InHC4` handles at most  $m$  constraints one by one. The procedure `InHC4R` applies at most  $k$  interval evaluations in time  $O(t)$  each during the backward projection phase, and  $k$  times a constant number (between one and four) calls to the procedure `MonoMaxInnerBox` during the top-down projection phase. When applied to a binary basic monotonic mathematical operator, the complexity of `MonoMaxInnerBox` is  $O(t)$  because it amounts to two iterations (on the two variables), each dominated by an interval evaluation of the basic operator.  $\square$

In contrast to `InnerPolytope`, observe that the worst-case complexity of `InHC4` is not reached when `InHC4R` fails to handle a constraint, since the loop on all the constraints is then interrupted. Therefore, the less chances `InHC4` has to extract an inner box (because the outer box is large compared to the inner subspace), the fewer constraints are handled by `InHC4`, and the shorter is the runtime needed.

## 6 Experiments

These two upper bounding algorithms have been implemented in our interval B&B `IbexOpt`. `IbexOpt` [27] is implemented in `Ibex` (Interval Based EXplorer) and enriches this C++ library devoted to interval solving [8].

At each node of the B&B, `IbexOpt` is called with our best operators for reducing the search space and improving the lower bound of the objective function:

– **Constraint programming contraction:**

The `ACID(Mohc)` operator is an adaptive version of CID [28] using `Mohc` [1] as basic contractor. `Mohc` is a state-of-the-art *constraint propagation* algorithm that exploits the monotonicity of constraints to better contract the current box. `Mohc` can be viewed as an improvement of the HC4 constraint propagation algorithm.

– **Contraction and lower bounding using a polyhedral convexification of the system:**

The operator `X-Newton` uses the dual form of (1) to contract the search space and improve the lower bound [2].

Most problems were solved using as bisection heuristic a variant of Kearfott’s *Smear* function described in [27]. Only a few problems in the test achieved in Section 6.1 were solved using the round robin bisection heuristic (denoted by `rr` in Table 2).

For upper bounding the cost, `IbexOpt` calls the `InnerPolytopeUB` and `InHC4UB` procedures described in this paper at each iteration/node of the B&B.

Note that the first version of `IbexOpt` was implemented in the first semester of year 2011, with the version 1.19 of `Ibex`, and published in [27]. We show in the experiments below three variants of `IbexOpt` with different features: the first version in `Ibex` 1.19, the latest version in `Ibex` 2.0, and an intermediary version in `Ibex` 1.20 (the last release of the version 1 of `Ibex`). The main features distinguishing these three variants of `IbexOpt` are summarized in Table 1.

**Table 1** Main changes in different versions of `IbexOpt`

Ibex(Opt) version	1.19	1.20	2.0
Constraint programming operator	<code>Mohc</code>	<code>ACID(Mohc)</code>	<code>ACID(HC4)</code>
Polyhedral convexification	lowerbounding with <code>X-Newton</code>	lb and contraction with <code>X-Newton</code>	lb and contraction with <code>X-Newt.</code> and affine arithmetic
Inner Polytope expansion point	$\underline{x}$	$\underline{x}$	random corner

Note that the `Mohc` constraint propagation algorithm is not yet reimplemented in `Ibex` 2.0, and using `ACID(Mohc)` instead of `ACID(HC4)` will improve the current strategy. Following studies reported in [2], the `X-Newton` (in fact `X-Taylor`) polyhedral convexification method is better exploited when  $2n + 1$  calls to a linear programming solver improves both the lower bound and the  $2n$  variable interval bounds. In addition, two hyperplanes are built per inequality in the latest version of the operator (see [2]). Finally, randomly choosing the

expansion point of the inner Taylor form at each node of the B&B slightly improves the results (compared to choosing always a same corner, e.g.,  $\underline{x}$  in (1)). `IbexOpt` 2.0 and IBBA techniques are currently merging, allowing the latest version of `IbexOpt` to embed affine arithmetic (thanks to Jordan Ninin).

### 6.1 Benefits brought by our upperbounding heuristics

The purpose of this section is to compare our algorithms for extracting inner regions (`InnerPolytopeUB` and `InHC4UB`) to a more basic inner test based on constraint inversion [4]. This test consists in reversing the inequality signs and applying `HC4-Revise` on every negated constraint. If the box  $[x]^{out}$  is each time discarded, one can conclude that every negated constraint contains no solution point in  $[x]^{out}$ , i.e.,  $[x]^{out}$  is entirely feasible.

To this end, we have set up a variant of our optimizer, called `IbexOpt0`, where the upper bounding is simplified as follows:

- `InnerPolytope` is not called.
- Only a simplified version of Algorithm 2 is called. In this version, the call to `InHC4` is removed. Instead, a call to the *inner test* is carried out. This test is a sufficient condition answering true if the handled box  $[x]^{out}$  is inner.

If the test fails, one resorts to random probing, as described in Algorithm 2. `IbexOpt` and `IbexOpt0` were implemented in Ibex 1.20 (see Table 1).

We made the comparison on a sample of instances issued from the series 1 of the COCONUT constrained global optimization benchmark. Equations  $h_k(x) = 0$  are relaxed by inequalities  $-\epsilon_{eq} \leq h_k(x) \leq \epsilon_{eq}$ , with  $\epsilon_{eq} = 1.e-8$ . The benchmark selection protocol is the following. We have selected the 59 systems solved in a runtime ranging from 1 second to 1 hour by `IbexOpt` or `IbexOpt0` with a standard computer having a 3 GHz Pentium processor. `IbexOpt` and `IbexOpt0` were implemented in Ibex 1.20 (see Table 1).

The name and number of variables of every system in the selected sample appear in Table 2.

The performance comparison between `IbexOpt` and `IbexOpt0` appears in Table 3 and Fig. 7.

## Results

This experiment highlights the significant benefits of our upper bounding, compared to simple probing and inner tests (based on constraint inversion) in every explored outer box. A loss in performance of 31% has been observed in only one instance whereas a speedup of at least a factor 2 has been observed on 33 systems. Furthermore, `IbexOpt0` was not able to solve 10 of the 59 selected systems: it reached the timeout in 1 system and raised a memory overflow in 9 systems.

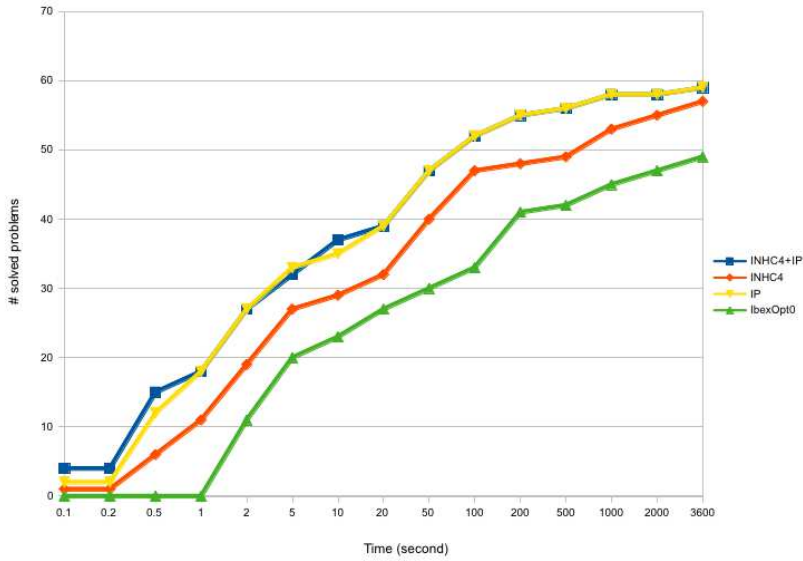
**Table 2** Sample of 59 systems selected in the serie 1 of the COCONUT benchmark.

name	$n$	name	$n$	name	$n$
alkyl (rr)	14	ex6.1.4	6	ex9.2.6	16
bearing	14	ex6.2.6	3	ex14.1.2	6
ex2.1.3	13	ex6.2.8	3	ex14.1.6	9
ex2.1.5	10	ex6.2.9	4	ex14.1.7	10
ex2.1.6	10	ex6.2.10	6	ex14.2.1	5
ex2.1.7	20	ex6.2.11	3	ex14.2.3	6
ex2.1.8	24	ex6.2.12	4	ex14.2.4	6
ex2.1.9	10	ex6.2.14	4	ex14.2.6	5
ex2.1.10	20	ex7.2.1	7	ex14.2.7	6
ex3.1.1	8	ex7.2.3	9	haverly	12
ex3.1.3	6	ex7.2.7 (rr)	4	hhfair	28
ex5.2.2.c1	9	ex7.2.8 (rr)	8	himmel11	9
ex5.2.2.c2	9	ex7.2.9 (rr)	10	himmel16	18
ex5.2.2.c3	9	ex7.3.4	12	house	8
ex5.2.4	7	ex7.3.5	13	hydro	30
ex5.3.2	22	ex8.1.8	6	immun (rr)	21
ex5.4.2	8	ex8.5.1	6	launch	38
ex5.4.3	16	ex8.5.2	6	meanvar	7
ex6.1.1	8	ex8.5.3	5	process	10
ex6.1.3	12	ex8.5.6	6		

**Table 3** Gains obtained by different optimizers  $X$  (IbexOpt, InHC4, IP) w.r.t. IbexOpt0. IP denotes a variant of the optimizer calling only InnerPolytopeUB at each iteration. InHC4 denotes a variant of the optimizer calling only InHC4UB at each iteration. IbexOpt=IP+InHC4 calls InnerPolytopeUB and InHC4UB. The gain is defined by  $\frac{time(IbexOpt0)}{time(X)}$ . For each line (gain range), the number of problems obtaining that gain is reported for the different optimizers. The penultimate line reports the number of systems successfully handled by  $X$  but which induce a memory overflow with IbexOpt0.

Gain	IbexOpt	InHC4	IP
< 0.69	0	0	0
0.69 – 0.9	1	4	2
0.9 – 1	2	2	2
1 – 1.1	0	11	0
1.1 – 2	14	13	13
2 – 10	19	15	22
10 – 100	11	3	8
> 100	3	2	3
Memory overflow (MO) with IbexOpt0	9	7	9
Solved within the timeout	59	57	59

InnerPolytope seems more useful than InHC4, but endowing a B&B with InnerPolytope and InHC4 together is more robust and shows a better performance than using each individually.



**Fig. 7** Performance profile. A point on a curve indicates the number of systems solved within the CPU time in abscissa by the corresponding optimizer.

## Qualitative study

Several qualitative analyses were conducted on the systems to better understand them individually and also to discover some general trends of our upper bounding heuristics.

A first attempt was to determine which of the two inner region extraction heuristics is the most useful in every system. To measure this, we counted the number of times `InHC4UB` and `InnerPolytopeUB` improved the upper bound. No general conclusion was drawn because the result does depend on every instance.

We also measured the mean size of outer boxes in which the algorithms succeed in extracting an inner region. Again, no definite trend was observed, but it appears that `InHC4UB` generally improves the upper bound in boxes that are larger than boxes where `InnerPolytopeUB` does. This would confirm that an interval Taylor form provides a good approximation of a non-convex function in a small box handled at the bottom of the search tree.

We finally observed a greater variability in runtime when `IbexOpt` is called with `InHC4UB` only than with `InnerPolytopeUB` only. (We tried 10 runs with different seeds for the random number generator.) This is due to the random choices made in the cases 2, 3 and 4 of `InHC4UB` (in the `MonoMaxInnerBox` procedure).

## 6.2 Comparison with other global optimizers

We conclude experiments with a comparison between six competitors belonging to the three types of deterministic branch & bounds for constrained global optimization (over the reals) introduced in Section 2:

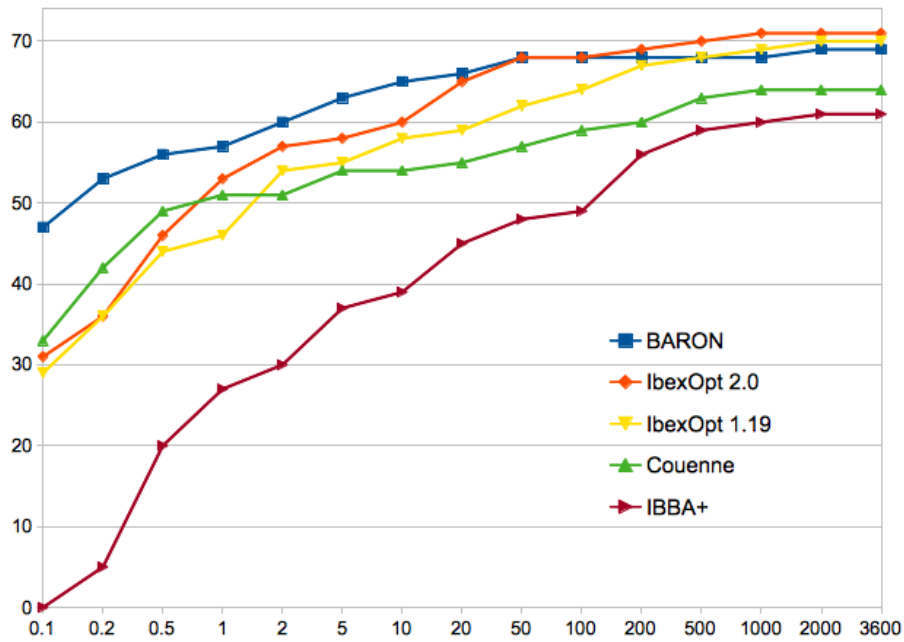
- **Baron** [26] and **Couenne** [3] cannot guarantee their results (see Section 2). In addition, **Couenne** rewrites the whole system using a DAG-based representation of the expressions where some common sub-expressions are detected and synthesized. The equations in this DAG are relaxed by two inequalities each, thus making the overall relaxation larger than with the original system.
- **IbexOpt** and **IBBA** return a floating-point vector guaranteed to be feasible in a system where the equations are relaxed. Two versions of **IbexOpt** are tested: the first one (**Ibex** 1.19) and the latest one (**Ibex** 2.0).
- **Icos** and **GlobSol** rigorously handle the global optimization problem under inequality and equality constraints (see Definition 2).

The rigorous answer of **Icos** and **GlobSol** is very interesting, but these interval optimizers are not competitive at all with the others in terms of performance. They show a loss of performance of several orders of magnitude compared to **Baron** or **IbexOpt** on many difficult instances. Thus, the results do not appear in the performance profile. Tables 2 and 3 in the first paper about **IbexOpt** [27] show the results obtained by **Icos** and **GlobSol** on 32 instances of the above sample.

The sample of instances used in the performance profile shown in Fig. 8 comprises the 74 instances tested by Ninin et al. [22] and reused in our AAI article [27]. This sample allows a comparison with **IBBA** [22]. All the competitors used the same precision parameters (i.e.,  $1e-8$  for the cost and the relaxation of equations). Most of the competitors were run on the same computer (Intel X86, 3 GHz). **Baron** was launched on the Neos server (see [www.neos-server.org/neos/](http://www.neos-server.org/neos/)) also on a X86, thus making the comparison rather fair. (Other experiments showed that the difference in CPU time between both computers is about 10%.) We can observe that **Baron** version 12 (June 2013) is generally the most efficient optimizer, but the difference with **IbexOpt** 2.0 is small, especially after 1 second of CPU time. Note that **IbexOpt** 2.0 solves two more instances than **Baron** in one hour. In particular, the system **ex7\_2.3** cannot be solved by **Baron** within the time limit of 3600 seconds, while this system is solved in less than 100 seconds by **IbexOpt** 2.0.

**IbexOpt** compares favorably with **Couenne** version 0.4 on this sample. It is worthwhile noting **Couenne** answers that 4 instances have no feasible points (**ex3\_1.1**, **ex5\_2.4**, **ex7\_3\_1**, **ex14\_1.9**). This underlines that the lack of rigor is not a theoretical drawback but does lead to failures in practice.

**Baron** and **Couenne** seem better than **IbexOpt** and **IBBA** on the most simple instances, in part because they can solve some of them during a pre-processing phase. **IbexOpt** and **IBBA** are not endowed with these pre-processing tools.



**Fig. 8** Performance profile. For a given strategy, a point  $(t, p)$  on the corresponding curve indicates that  $p$  among the 74 systems are solved in less than  $t$  seconds.

However, in 1 or 2 seconds, `IbexOpt` can solve the same number of systems as `Couenne`, while `IbexOpt 2.0` reaches the performance of `Baron` in 50 seconds.

`IbexOpt` is (one order of magnitude) more efficient than `IBBA` and we know that upperbounding with inner regions mainly explains this gain in performance (see [27]).

## 7 Conclusion

We have proposed in this paper a new upperbounding policy for systems with inequality constraints (or relaxed equalities). The two proposed heuristics (`InnerPolytope` and `InHC4`) first extract an inner (entirely feasible) region and then select a good (or best) point inside the extracted inner region for updating the upper bound with its cost. We have obtained very good results on a representative sample of medium-sized instances proposed in the COCONUT benchmark suite. `InnerPolytope` obtains the best results on the sample, although using both `InnerPolytope` and `InHC4` renders the upperbounding phase more robust. Overall, endowed with these upperbounding features, `IbexOpt` compares favorably with deterministic global optimizers found in the literature, namely `Couenne`, `IBBA`, `Icos`, `GlobSol`. `Baron` remains more efficient than `IbexOpt`, in particular on easy instances or on polynomial ones.

This is not the case for systems with non polynomial operators (division, *sine*, *log*, etc).

It is worthwhile noting that our upperbounding does not use any local minimization approach. As shown in Section 5, our heuristics are not costly and are thus used at each node of the interval B&B. In other deterministic optimizers, upperbounding with local minimization is often costly because of the heavy generation of the Lagrangian relaxation. Therefore, these optimizers generally do not call this process at each node of the B&B. We believe that both approaches are complementary, and integrating them together is an interesting line of research.

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