Solving Polynomial Systems Using a Branch and Prune Approach

P. Van Hentenryck[1]
D. McAllester[2]
D. Kapur[3]

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[1]Dept.of Computer Science,Brown University Providence, RI 02912
[2]MIT AI Lab, 545 Technology Square Cambridge, MA
[3]SUNY at Albany, Dept of Computer Science Albany, NY 12222

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P. Van Hentenryck
Brown University
Box 1910
Providence, RI 02912
pvh@cs.brown.edu

D. McAllester
MIT AI Lab
Technology Square, 545
Cambridge, USA
dam@ai.mit.edu

D. Kapur
SUNY at Albany
Dep. of Computer Science
Albany, NY-12222
kapur@cs.albany.edu

Abstract

This paper presents `Newton`, a branch & prune algorithm to find all isolated solutions of a system of polynomial constraints. `Newton` can be characterized as a global search method which uses intervals for numerical correctness and for pruning the search space early. The pruning in `Newton` consists in enforcing at each node of the search tree a unique local consistency condition, called box-consistency, which approximates the notion of arc-consistency well-known in artificial intelligence. Box-consistency is parametrized by an interval extension of the constraint and can be instantiated to produce Hansen-Segupta narrowing operator (used in interval methods) as well as new operators which are more effective when the computation is far from a solution. `Newton` has been evaluated on a variety of benchmarks from kinematics, chemistry, combustion, economics, and mechanics. On these benchmarks, it outperforms the interval methods we are aware of and compares well with state-of-the-art continuation methods. Limitations of `Newton` (e.g. a sensitivity to the size of the initial intervals on some problems) are also discussed. Of particular interest is the mathematical and programming simplicity of the method.

1 Introduction

Many applications in science and engineering (e.g. chemistry, robotics, economics, mechanics) require finding all isolated solutions to a system of polynomial constraints over real numbers. This problem is difficult due to its inherent computational complexity (i.e., it is NP-hard) and due to the numerical issues involved to guarantee correctness (i.e., finding all solutions) and to ensure termination. Several interesting methods have been proposed in the past for this task, including two fundamentally different methods: interval methods (e.g. [13, 5, 4, 8]) and continuation methods (e.g. [18, 26]). Continuation methods have been shown to be effective for problems for which the total degree is not too high, since the number of paths explored depends on the estimation of the number of solutions. Interval methods are generally robust but tend to be slow.

The purpose of this paper is to propose and to study a novel algorithm called `Newton`. From a user standpoint, `Newton` receives as input a system of polynomial constraints over, say, variables $x_1, \ldots, x_n$ and a box, i.e., an interval tuple $\langle I_1, \ldots, I_n \rangle$ specifying the initial range of these variables; it returns a set of boxes of specified accuracy containing all solutions.

Operationally, `Newton` is a branch & prune algorithm which was inspired by the traditional branch and bound approach used to solve combinatorial optimization problems. `Newton` uses intervals to address the two fundamental problems listed above. Numerical reliability is obtained by evaluating functions over intervals using outward rounding (as in interval methods). The complexity issue is addressed by using constraints to reduce the intervals early in the search. The pruning in `Newton` is achieved by enforcing a unique local consistency condition, called box-consistency, at each node of the search tree. Box-consistency is an approximation of arc-consistency, a notion well-known in artificial intelligence [10, 12] and used to solve discrete combinatorial problems in several systems (e.g., [23, 24]). Box-consistency is parametrized by an interval extension operator for the constraint and can be instantiated to produce various narrowing operators. In particular, box-consistency on the Taylor extension of the constraint produces a generalization of Hansen-Segupta operator [5], well-known in interval methods. In addition, box-consistency on the natural extension produces narrowing operators which are more effective when the algorithm is not near a solution. `Newton` has the following properties:

- **Correctness:** `Newton` finds all isolated solutions to the system in the following sense: if $\langle v_1, \ldots, v_n \rangle$ is a solution, then `Newton` returns at least one box $\langle I'_1, \ldots, I'_n \rangle$ such that $v_i \in I_i$ $(1 \leq i \leq n)$. In addition, `Newton` may guarantee the existence of a unique solution in some or all the boxes in the result.

- **Termination:** `Newton` always terminates in finite time.

- **Effectiveness:** `Newton` has been evaluated on a variety of benchmarks from kinematics, chemistry, combustion, economics, and mechanics. It outperforms the interval methods we are aware of and compares well with state-of-the-art continuation methods on many problems. Interestingly, `Newton` solves the Broyden banded function problem [5] and Moré-Cosnard discretization of a nonlinear integral equation [16] for several hundred variables.

- **Simplicity and Uniformity:** `Newton` is based on simple mathematical results and is easy to use and to implement. It is also based on a single concept: box-consistency.

The rest of this paper is organized as follows. Section 2 gives an overview of the approach. Section 3 contains the preliminaries. Section 4 presents an abstract version of the branch & prune algorithm. Section 5 discusses the implementation of the box-consistency. Section 6 describes the experimental results. Section 7 discusses related work and the development of the ideas presented here. Section 8 concludes the paper.

2 Overview of The Approach

As mentioned, `Newton` is a global search algorithm which solves a problem by dividing it into subproblems which are solved recursively. In addition, `Newton` is a branch & prune algorithm which means that it is best viewed as an iteration of two steps

1. pruning the search space;

2. making a nondeterministic choice to generate two subproblems

until one or all solutions to a given problem are found.

The pruning step is responsible to make sure that some local consistency conditions are satisfied. It consists of reducing the intervals associated with the variables so that every constraint appears to be locally consistent. The local consistency condition of `Newton` is called box-consistency, an approximation of arc-consistency, a notion well-known in artificial intelligence [10, 12] and used in many systems (e.g. [24, 25, 22]) to solve discrete combinatorial search problems. Informally speaking, a constraint is arc-consistent if for each value in the range of a variable there exist values in the ranges of the other variables such that the constraint is satisfied. `Newton` approximates arc-consistency which cannot be computed on real numbers in general.

The pruning step either fails, showing the absence of solution in the intervals, or succeeds in enforcing the local consistency condition. Sometimes, local consistency also implies global consistency as in the case of the Broyden banded function, i.e.

$$f_i(x_1, \ldots, x_n) = x_i(2 + 5x_i^2) + 1 - \sum_{j \in J_i} x_j(1 + x_j) \quad (1 \leq i \leq n)$$

where $J_i = \{j \mid j \neq i \;\&\; max(1, i-5) \leq j \leq min(n, i+1)\}$. The pruning step of `Newton` solves this problem in essentially linear time for initial intervals of the form $[-10^8, 10^8]$ and always proves the existence of a solution in the final box. However, in general, local consistency does not imply global consistency either because there are multiple solutions or simply because the local consistency condition is too weak. Consider the intersection of a circle and of a parabola:

$$\begin{cases} x_1^2 + x_2^2 = 1 \\ x_1^2 - x_2 = 0 \end{cases}$$

with initial intervals in $[-10^8, 10^8]$. The pruning step returns the intervals

$$\begin{aligned} x_1 &\in [-1.0000000000012430057, +1.0000000000012430057] \\ x_2 &\in [-0.0000000000000000000, +1.0000000000012430057] \end{aligned}$$

with 8 digits of accuracy. The pruning is obtained by a simple reasoning about the intervals. For instance, from the second equation, it is easily deduced that $x_2 \geq 0$. From the first equation, `Newton` deduces that x_1^2 is not more than 1 and thus that x_1 is in [-1,1]. The same reasoning applies to x_2. `Newton` then uses the second equation to conclude that x_2 is in [0,1]. Branching on x_1 produces the intervals

$$\begin{aligned} x_1 &\in [-1.0000000000012430057, +0.0000000000000000000] \\ x_2 &\in [-0.0000000000000000000, +1.0000000000012430057] \end{aligned}$$

Further pruning is obtained by taking the Taylor extension of the polynomials in the above equations around $(-0.5, 0.5)$, the center of the above box and by conditioning the system to obtain by bound reasoning

$$\begin{aligned} x_1 &\in [-1.0000000000000000000, -0.6049804687499998889] \\ x_2 &\in [+0.3821067810058591529, +0.8433985806150308129]. \end{aligned}$$

Simple bound reasoning on the original constraints then leads to the solution

$$\begin{aligned} x_1 &\in [-0.7861513777574234974, -0.7861513777574231642] \\ x_2 &\in [+0.6180339887498946804, +0.6180339887498950136]. \end{aligned}$$

Backtracking on the choice for x_1 produces the intervals

$$\begin{aligned} x_1 &\in [-0.0000000000000000000, +1.0000000000012430057] \\ x_2 &\in [-0.0000000000000000000, +1.0000000000012430057] \end{aligned}$$

and to the second solution

$$x_1 \in [+0.78615137775742316\,42, +0.78615137775742338\,64]$$
$$x_2 \in [+0.61803398874989468\,04, +0.61803398874989501\,36].$$

Note that, in this case, `Newton` makes the smallest number of choices to isolate the solutions.[1] To conclude this motivating section, let us illustrate `Newton` on a larger example which describes the inverse kinematics of an elbow manipulator [7]:

$$\begin{cases} s_2c_5s_6 - s_3c_5s_6 - s_4c_5s_6 + c_2c_6 + c_3c_6 + c_4c_6 = 0.4077 \\ c_1c_2s_5 + c_1c_3s_5 + c_1c_4s_5 + s_1c_5 = 1.9115 \\ s_2s_5 + s_3s_5 + s_4s_5 = 1.9791 \\ c_1c_2 + c_1c_3 + c_1c_4 + c_1c_2 + c_1c_3 + c_1c_2 = 4.0616 \\ s_1c_2 + s_1c_3 + s_1c_4 + s_1c_2 + s_1c_3 + s_1c_2 = 1.7172 \\ s_2 + s_3 + s_4 + s_2 + s_3 + s_2 = 3.9701 \\ s_i^2 + c_i^2 = 1 \qquad (1 \le i \le 6). \end{cases}$$

and assumes that the initial intervals are in $[-10^8, 10^8]$ again. The pruning step returns the intervals

$$\begin{array}{l} [-1.0000000000000000000, +1.0000000000000000000] \\ [-1.0000000000000000000, +1.0000000000000000000] \\ [+0.3233666666666665800, +1.0000000000000000000] \\ [-1.0000000000000000000, +1.0000000000000000000] \\ [-0.0149500000000000189, +1.0000000000000000000] \\ [-1.0000000000000000000, +1.0000000000000000000] \\ [-0.0209000000000001407, +1.0000000000000000000] \\ [-1.0000000000000000000, +1.0000000000000000000] \\ [+0.6596999999999998420, +1.0000000000000000000] \\ [-0.7515290480087772896, +0.7515290480087772896] \\ [-1.0000000000000000000, +1.0000000000000000000] \\ [-1.0000000000000000000, +1.0000000000000000000] \end{array}$$

showing already some interesting pruning. After exactly 12 branchings and in less than a second, `Newton` produces the first box with a proof of existence of a solution in the box.

3 Preliminaries

In this section, we review some basic concepts needed for this paper, including interval arithmetic and the representation of constraints. More information on interval arithmetic can be found in many places (e.g., [1, 5, 4, 13, 14]). Our definitions are slightly non-standard.

[1] This example can also be solved by replacing x_1^2 in the first equation by x_2 to obtain a univariate constraint in x_2 which can be solved independently. However, this cannot always be done and the discussion here is what `Newton` would do, without making such optimizations.

3.1 Interval Arithmetic

We consider $\Re^{\infty} = \Re \cup \{-\infty, \infty\}$ the set of real numbers extended with the two infinity symbols and the natural extension of the relation $<$ to this set. We also consider a finite subset $\mathcal{F}$ of $\Re^{\infty}$ containing $-\infty, \infty, 0$. In practice, $\mathcal{F}$ corresponds to the floating-point numbers used in the implementation.

Definition 1 [Interval] An interval $[a, b]$ with $a, b \in \mathcal{F}$ is the set of real numbers

$$\{r \in \Re \mid a \leq r \leq b\}.$$

The set of intervals is denoted by $\mathcal{I}$ and is ordered by set inclusion.

Definition 2 [Approximation] Let S be a subset of $\Re$. The approximation of S, denoted by $\overline{S}$ or $box\{S\}$, is the smallest interval I such that $S \subseteq I$. We often write $\overline{r}$ instead of $\overline{\{r\}}$ for $r \in \Re$. We also write $I_1 \uplus I_2$ to denote $box\{I_1 \cup I_2\}$.

In the following, we denote real numbers by the letters r, v, $\mathcal{F}$-numbers by the letters a, b, l, m, u, intervals by the letter I, real functions by the letters f, g and interval functions by the letters F, G, all possibly subscripted. We use a^+ (resp. a^-) to denote the smallest (resp. largest) $\mathcal{F}$-number strictly greater (resp. smaller) than the $\mathcal{F}$-number a. To capture outward rounding, we use $\lceil r \rceil$ (resp. $\lfloor r \rfloor$) to return the smallest (resp. largest) $\mathcal{F}$-number greater (resp. smaller) or equal to the real number r. We also use $\vec{I}$ to denote a box $\langle I_1, \ldots, I_n \rangle$ and $\vec{r}$ to denote a tuple $\langle r_1, \ldots, r_n \rangle$. Finally, we use the following notations.

$$\begin{aligned}
&left([l, u]) = l \\
&right([l, u]) = u \\
&center([l, u]) = \lfloor (l + u)/2 \rfloor
\end{aligned}$$

The fundamental concept of interval arithmetic is the notion of interval extension.

Definition 3 [Interval Extension] $F : \mathcal{I}^n \rightarrow \mathcal{I}$ is an interval extension of $f : \Re^n \rightarrow \Re$ iff

$$\forall I_1 \ldots I_n : r_1 \in I_1, \ldots, r_n \in I_n \Rightarrow f(r_1, \ldots, r_n) \in F(I_1, \ldots, I_n).$$

An interval relation $C : \mathcal{I}^n \rightarrow Bool$ is an interval extension of a relation $c : \Re^n \rightarrow Bool$ iff

$$\forall I_1 \ldots I_n : r_1 \in I_1, \ldots, r_n \in I_n \Rightarrow [c(r_1, \ldots, r_n) \Rightarrow C(I_1, \ldots, I_n)].$$

Example 1 The interval function $\oplus$ defined as

$$[a_1, b_1] \oplus [a_2, b_2] = [\lfloor a_1 + a_2 \rfloor, \lceil b_1 + b_2 \rceil]$$

is an interval extension of addition of real numbers. The interval relation $\approx$ defined as

$$I_1 \approx I_2 \;\Leftrightarrow\; (I_1 \cap I_2 \neq \emptyset)$$

is an interval extension of the equality relation on real numbers.

It is important to stress that a real function (resp.) can be extended in many ways. For instance, the interval function $\oplus$ is the most precise interval extension of addition (i.e., it returns the smallest possible interval containing all real results) while a function always returning $[-\infty, \infty]$ would be the least accurate.

In the following, we assume fixed interval extensions for the basic real operators $+, -, \times$ and exponentiation (for instance, the interval extension of $+$ is defined by $\oplus$) and the basic real relations $=, \geq$. In addition, we overload the real symbols and use them for their interval extensions. Finally, we denote relations by the letter c possibly subscripted, interval relations by the letter C possibly subscripted. Note that constraints and relations are used as synonyms in this paper.

3.2 Unions of Intervals

Even though many basic real operators can be naturally extended to work on intervals, division creates problems if the interval used for dividing includes 0. A tight extension of division to intervals can be best expressed if its result can be a union of intervals. Assuming that $c \leq 0 \leq d$ and $c < d$, $[a, b]/[c, d]$ is defined as follows:

$$
\begin{array}{ll}
[\lfloor b/c \rfloor, \infty] & \text{if } b \leq 0 \text{ and } d = 0 \\
[-\infty, \lceil b/d \rceil] \cup [\lfloor b/c \rfloor, \infty] & \text{if } b \leq 0 \text{ and } c < 0 < d \\
[-\infty, \lceil b/d \rceil] & \text{if } b \leq 0 \text{ and } c = 0 \\
[-\infty, \infty] & \text{if } a < 0 < b \\
[-\infty, \lceil a/c \rceil] & \text{if } a \geq 0 \text{ and } d = 0 \\
[-\infty, \lceil a/c \rceil] \cup [\lfloor b/c \rfloor, \infty] & \text{if } a \geq 0 \text{ and } c < 0 < d \\
[\lfloor a/d \rfloor, \infty] & \text{if } a \geq 0 \text{ and } c = 0.
\end{array}
$$

The case where $0 \notin [c, d]$ is easy to define. Note also that other operations such as addition and subtraction can also be extended to work with unions of intervals.

A typical use of unions of intervals in interval arithmetic is to take the intersection of an interval I with the result of an operation of the form $I_1 - I_2/I_3$. To increase precision, $I_1 - I_2/I_3$ is computed with unions of intervals. The result is then intersected with I and is possibly approximated to return a single interval.

3.3 Constraint Representations

It is well-known that different computer representations of a real function produce different results when evaluated with floating-point numbers on a computer. As a consequence, the way constraints are written may have an impact on the behaviour on the algorithm. For this reason, a constraint or a function in this paper is considered to be an expression written in terms of the real functional and relational symbols. This can be formalized by assuming that all constraints used in this paper are written in a language whose abstract syntax is specified by the following grammar:

$$
\begin{array}{lll}
c & \in & \mathit{Constraint} \\
f & \in & \mathit{Function} \\
x_i & \in & \mathit{RealVariables} = \{x_1, \ldots, x_n\} \\
q & \in & \mathcal{Q} \\
n & \in & \mathcal{N}
\end{array}
$$

$$
\begin{array}{lll}
c & ::= & f = 0 \mid f \geq 0 \\
f & ::= & q \mid x_i \mid f + f \mid f - f \mid f \times f \mid f^n \mid (f)
\end{array}
$$

It is easy to extend the language to accommodate more functions (e.g. *sin, cos, ...*). Note that we assume for simplicity that all constraints are written using a finite (but arbitrary large) set of variables $\{x_1, \ldots, x_n\}$. Let e be a tuple $(r_1, \ldots, r_n)$ and $e_{|i}$ be r_i $(1 \leq i \leq n)$. The semantics of the language is given by the following semantic functions whose signatures are

$$
\begin{array}{l}
\mathcal{S}_c : \mathit{Constraint} \rightarrow \Re^n \rightarrow \mathit{Bool} \\
\mathcal{S}_f : \mathit{Function} \rightarrow \Re^n \rightarrow \Re
\end{array}
$$

and whose semantic equations are specified as follows:

$$
\begin{array}{lll}
\mathcal{S}_c[\![f = 0]\!] & = & \lambda e.\ \mathcal{S}_f[\![f]\!]e \ = \ 0 \\
\mathcal{S}_c[\![f \geq 0]\!] & = & \lambda e.\ \mathcal{S}_f[\![f]\!]e \ \geq \ 0 \\
\mathcal{S}_f[\![q]\!] & = & \lambda e.\ q \\
\mathcal{S}_f[\![x_i]\!] & = & \lambda e.\ e_{|i} \\
\mathcal{S}_f[\![f_1 + f_2]\!] & = & \lambda e.\ \mathcal{S}_f[\![f_1]\!]e + \mathcal{S}_f[\![f_2]\!]e \\
\mathcal{S}_f[\![f_1 - f_2]\!] & = & \lambda e.\ \mathcal{S}_f[\![f_1]\!]e - \mathcal{S}_f[\![f_2]\!]e \\
\mathcal{S}_f[\![f_1 \times f_2]\!] & = & \lambda e.\ \mathcal{S}_f[\![f_1]\!]e \times \mathcal{S}_f[\![f_2]\!]e \\
\mathcal{S}_f[\![f^n]\!] & = & \lambda e.\ (\mathcal{S}_f[\![f]\!]e)^n \\
\mathcal{S}_f[\![(f)]\!] & = & \lambda e.\ \mathcal{S}_f[\![f]\!]e
\end{array}
$$

In the following, we often abuse notation and use f (resp. c) to denote $\mathcal{S}_f[\![f]\!]$ (resp. $\mathcal{S}_c[\![c]\!]$) and vice-versa. However, the meaning should be clear from the context. We also assume that interval functions and interval relations are defined using a similar abstract syntax and semantics except that real variables (i.e. x_i) are replaced by interval variables (i.e. X_i) and rational numbers by intervals. We use *CONSTRAINT* and *FUNCTION* to denote the set of interval constraints and functions. For simplicity of exposion, we restrict attention to equations. It is straightforward to generalize our results to inequalities (see Section 5.5).

4 The Branch & Prune Algorithm

This section describes the branch & prune algorithm `Newton`. Section 4.1 defines box-consistency, the key concept behing our algorithm. Section 4.2 shows how box-consistency can be instantiated to produce various pruning operators achieving various tradeoffs between accuracy and efficiency. Section 4.3 defines a conditioning operator used in `Newton` to improve the effectiveness of box-consistency. Section 4.4 specifies the pruning in `Newton`. Section 4.5 describes the algorithm. Recall that we assume that all constraints are defined over variables $x_1, \ldots, x_n$.

4.1 Box Consistency

Box-consistency [2] is an approximation of arc-consistency, a notion well-known in artificial intelligence [10] which states a simple local condition on a constraint c and the set of possible values for each of its variables, say $D_1, \ldots, D_n$. Informally speaking, a constraint c is arc-consistent if none of the D_i can be reduced by using projections of c.

Definition 4 [Projection Constraint] A projection constraint $\langle c, i\rangle$ is the association of a constraint c and of an index i ($1 \leq i \leq n$). Projection constraints are denoted by the letter P, possibly subscripted.

Definition 5 [Arc-Consistency] A projection constraint $\langle c, i\rangle$ is arc-consistent wrt $\langle D_1, \ldots, D_n\rangle$ iff $D_i = D_i \cap \{r_i \mid \exists r_1 \in D_1, \ldots, \exists r_{i-1} \in D_{i-1}, \ldots, \exists r_{i+1} \in D_{i+1}, \ldots, \exists r_n \in D_n : c(r_1, \ldots, r_n)\}$. A constraint c is arc-consistent wrt $\langle D_1, \ldots, D_n\rangle$ if each of its projections is arc-consistent wrt $\langle D_1, \ldots, D_n\rangle$. A system of constraints $\mathcal{S}$ is arc-consistent wrt $\langle D_1, \ldots, D_n\rangle$ if each constraint in $\mathcal{S}$ is arc-consistent wrt $\langle D_1, \ldots, D_n\rangle$.

Arc-consistency cannot be computed in general when working with real numbers and polynomial constraints and simple approximations to capture machine precision are very expensive to compute. For instance, a simple approximation of arc-consistency consists in working with intervals and approximating the set computed by arc-consistency to return an interval, i.e.

$$I_i = box\{I_i \cap \{\ r_i \mid \exists r_1 \in I_1, \ldots, \exists r_{i-1} \in I_{i-1}, \ldots, \exists r_{i+1} \in I_{i+1}, \ldots, \exists r_n \in I_n : c(r_1, \ldots, r_n)\ \}\}.$$

This condition, used in systems like [19, 3], is easily enforced on simple constraints such as

$$x_1 = x_2 + x_3, \quad x_1 = x_2 - x_3, \quad x_1 = x_2 \times x_3$$

but it is also computationally very expensive for complex constraints with multiple occurrences of the same variables. Moreover, decomposing complex constraints into simple constraints entails a substantial loss in pruning, making this approach unpractical on many applications. See [2] for experimental results on this approach and their comparison with the approach presented in this paper.

The notion of box-consistency introduced in [2] is a coarser approximation of arc-consistency which provides a much better trade-off between efficiency and pruning. It consists in replacing the existential quantification in the above condition by the evaluation of an interval extension of the constraint on the intervals of the existential variables. Since different interval extensions will produce different results, it is necessary and useful to parametrize the definition of box-consistency with an operator which maps a constraint into one of its extensions.

Definition 6 [Extension Operator] An extension operator is a function of signature

$$Constraint \rightarrow CONSTRAINT$$

Definition 7 [Box-Consistency] A projection constraint $\langle c, i\rangle$ is box-consistent wrt $\vec{I} = \langle I_1, \ldots, I_n\rangle$ and an extension operator IE iff

$$IE(c)(I_1, \ldots, I_{i-1}, [l, l^+], I_{i+1}, \ldots, I_n) \ \wedge \ IE(c)(I_1, \ldots, I_{i-1}, [u^-, u], I_{i+1}, \ldots, I_n).$$

where $l = left(I_i)$ and $u = right(I_i)$ A constraint is box-consistent wrt $\vec{I}$ and IE if each of its projections is box-consistent wrt $\vec{I}$ and IE. A system of constraints is box-consistent wrt $\vec{I}$ and IE iff each constraint in the system is box-consistent wrt $\vec{I}$ and IE.

Intuitively speaking, the above condition states that the ith interval cannot be pruned further using the unary interval constraint obtained by replacing all variables but x_i by their intervals, since the boundaries satisfy the unary constraint. Note also that the above condition is equivalent to

$$I_i = box\{\ r_i \ \in \ I_i \mid IE(I_1, ..., I_{i-1}, \overline{r_i}, I_{i+1}, ..., I_n\ \}$$

which shows clearly that box-consistency is an approximation of arc-consistency.

4.2 Interval Extensions for Box Consistency

Box-consistency strongly depends on the extension operator *IE* and different choices of operators can produce very different (often incomparable) tradeoffs between pruning and computational complexity. In this section, we consider the three extension operators used in `Newton`: natural interval extension, distributed interval extension, and Taylor interval extension.

4.2.1 Natural Interval Extension

The easiest extension operator produces the natural interval extension of a constraint. Informally speaking, it consists in replacing each real number by an interval, each real variable by an interval variable, each real operation by its fixed interval extension. Formally, it is captured by the following definition.

Definition 8 [Natural Interval Extension] The natural interval extension of a constraint c, denoted by $NE(c)$ and of signature $NE : Constraint \rightarrow CONSTRAINT$ is defined inductively as follows:

$$
\begin{array}{lcl}
NE[\![f = 0]\!] & = & NE[\![f]\!] = \overline{0} \\
NE[\![q]\!] & = & \overline{q} \\
NE[\![x_i]\!] & = & X_i \\
NE[\![f_1 + f_2]\!] & = & NE[\![f_1]\!] + NE[\![f_2]\!] \\
NE[\![f_1 - f_2]\!] & = & NE[\![f_1]\!] - NE[\![f_2]\!] \\
NE[\![f_1 \times f_2]\!] & = & NE[\![f_1]\!] \times NE[\![f_2]\!] \\
NE[\![f^n]\!] & = & (NE[\![f]\!])^n \\
NE[\![(f)]\!] & = & NE[\![f]\!]
\end{array}
$$

The advantage of this extension is that it preserves the way constraints are written and hence users of the system can choose constraint representations particularly appropriate for the problem at hand. A very nice application where this extension is fundamental is the Moré-Cosnard discretization of a nonlinear integral equation (See Section 6.2). Using the natural extension allows users to minimize the problem of dependency of interval arithmetic and hence to increases precision.

4.2.2 Distributed Interval Extension

The second interval extension used by `Newton` does not preserve the way constraints are written but uses an distributed form of the constraints. The key advantage of this extension is that it allows the algorithm to enforce box-consistency by applying Newton interval method on univariate real functions. The real functions are derived from univariate interval constraints obtained by replacing all but one variable by their intervals. As a consequence, applying box-consistency will be particularly efficient, although the pruning may be weaker than for the natural extension due to the dependency problem of interval arithmetics.[2] Intuitively, the distributed interval extension should be viewed as a way to speed up the computation of box-consistency on the natural extension. However, it may happen that it gives more precision than the natural extension if users are not careful in stating their constraints.

[2]Note that it is not always necessary to go through the distributed form to obtain the above property but `Newton` adopts it for simplicity.

Definition 9 [Distributed Form] A constraint c is in (simplified) sum of products form

$$m_1 + \cdots + m_k = 0,$$

where each monomial m_i is of the form $qx_1^{e_1} \cdots x_n^{e_n}$ with $q \in \mathcal{Q}$ and $e_i \in \mathcal{N}$, is said to be in distributed form. Given a constraint c, we denote its distributed version by $DF(c)$.[3]

Definition 10 [Distributed Interval Extension] The distributed interval extension of a constraint c, denoted by $DE(c)$ and of signature $DE : \mathit{Constraint} \rightarrow \mathit{CONSTRAINT}$, is

$$\mathit{NE}(DF(c)).$$

4.2.3 Taylor Interval Extension Generator

The last interval extension we introduce is based on the Taylor expansion around a point. Instead of presenting a single extension, we present a generator of extensions, since it will be important to generate an extension for a box under consideration. The generator has signature

$$\mathcal{I}^n \rightarrow \mathit{Constraint} \rightarrow \mathit{CONSTRAINT}$$

and it assumes that the constraint which it is applied to is of the form $f = 0$ where f denotes a function which has continuous partial derivatives. Given these assumptions, the key idea behind the operator is to apply a Taylor expansion of the function around the center of the box and to bound the rest of the series using the box.

Definition 11 [Taylor Interval Extension Generator] Let c be a constraint $f = 0$, f be a function with continuous partial derivatives, $\vec{I}$ be a box $(I_1, \ldots, I_n)$, and c_i be the center of I_i. The Taylor interval extension generator $TE(\vec{I})(c)(X_1, \ldots, X_n)$ is defined

$$\mathit{NE}(f)(\overline{c_1}, \ldots, \overline{c_n}) + \sum_{i=1}^{n} \mathit{DER}(f, i)(I_1, \ldots, I_n)\,(X_i - \overline{c_i}) \;\; = \;\; \overline{0}.$$

where $\mathit{DER}(f, i)$ returns an interval extension of $\frac{\partial f}{\partial x_i}$.

In the current version of our system, the operator DER of signature $(\mathit{Function} \times \mathcal{N}) \rightarrow \mathit{FUNCTION}$ is defined as $\mathit{NE}(D(f, i))$ where $D : (\mathit{Function} \times \mathcal{N}) \rightarrow \mathit{FUNCTION}$ is specified as follows:

$$\begin{array}{lcl}
D[\![q, i]\!] & = & 0 \\
D[\![x_i, i]\!] & = & 1 \\
D[\![x_j, i]\!] & = & 0 \quad (i \neq j) \\
D[\![f_1 + f_2, i]\!] & = & D[\![f_1, i]\!] + D[\![f_2, i]\!] \\
D[\![f_1 - f_2, i]\!] & = & D[\![f_1, i]\!] - D[\![f_2, i]\!] \\
D[\![f_1 \times f_2, i]\!] & = & f_1 \times D[\![f_2, i]\!] + f_2 \times D[\![f_1, i]\!] \\
D[\![f^n, i]\!] & = & n \times f^{n-1} \times D[\![f, i]\!] \\
D[\![(f), i]\!] & = & D[\![f, i]\!]
\end{array}$$

[3]The distributed version can easily be turned into a canonical representation for constraints.

4.3 Conditioning

It is interesting to note that box-consistency on the Taylor interval extension is closely related to Hansen-Segupta's operator [5], which is an improvement over Krawczyk's operator [8]. Hansen and Smith [6] also argued that these operators are more effective for a system $\{f_1 = 0, \ldots, f_n = 0\}$ wrt a box $\langle I_1, \ldots, I_n \rangle$ when the interval Jacobian

$$M_{ij} = DER(f_i, j)(I_1, \ldots, I_n) \; (1 \leq i, j \leq n)$$

is diagonally dominant, i.e.,

$$mig(M_{i,i}) \geq \sum_{j=1, j \neq i}^{n} mag(M_{i,j})$$

where

$$mig([l, u]) = min(\mid l \mid, \mid u \mid) \text{ and } mag([l, u]) = max(\mid l \mid, \mid u \mid).$$

They also suggest a conditioning which consists in multiplying the linear relaxation by a real matrix which is the inverse of the matrix obtained by taking the center of $M_{i,j}$. The resulting system is generally solved through Gauss-Seidel iterations, giving Hansen-Segupta's operator. `Newton` exploits this idea to improve the effectiveness of box-consistency on the Taylor interval extension. The conditioning of `Newton` is abstracted by the following definition.

Definition 12 [Conditioning] Let $S = \{f_1 = 0, \ldots, f_n = 0\}$. A conditioning of S is a system $S' = \{f'_1 = 0, \ldots, f'_n = 0\}$ where

$$f'_i = \sum_{k=1}^{n} A_{ik} f_k$$

where $A_{ik} \in \mathcal{Q}$.

In its present implementation, `Newton` uses a conditioning $cond(\{f_1 = 0, \ldots, f_n = 0\}, \vec{I})$ which returns a system $\{f'_1 = 0, \ldots, f'_n = 0\}$ such that

$$f'_i = \sum_{k=1}^{n} A_{ik} f_k$$

where

$$\begin{array}{lcl} M_{ij} & = & DER(f_i, j)(I_1, \ldots, I_n) \; (1 \leq i, j \leq n) \\ B_{ij} & = & center(M_{ij}) \\ A & = & \begin{cases} B^{-1} & \text{if } B \text{ is not singular} \\ I & \text{otherwise.} \end{cases} \end{array}$$

Note that the computation of the inverse of B is obtained by standard floating-point algorithms.

4.4 Pruning in `Newton`

We now describe the pruning of `Newton`. The key idea behind `Newton` is to apply box-consistency at each node of the search tree, i.e., `Newton` reduces the current intervals for the variables in such a way that the constraint system is box-consistent wrt the reduced intervals and no solution is removed. The pruning is performed by using narrowing operators deduced from the definition of box-consistency. These operators are used to reduce the interval of a variable using a projection constraint.

Definition 13 [Box-Narrowing] Let $\langle c, i\rangle$ be a projection constraint, $\langle I_1, \ldots, I_n\rangle$ be a box, and IE be a interval extension operator. The narrowing operator `BOX-NARROW` is defined as

$$\texttt{BOX-NARROW}(\langle c,i\rangle,\langle I_1,\ldots,I_n\rangle,IE) = \langle I_1,\ldots,I_{i-1},I,I_{i+1},\ldots,I_n\rangle$$

where I is defined as the largest set included in I_i such that $\langle c, i\rangle$ is box-consistent with respect to $\langle I_1, \ldots, I_{i-1}, I, I_{i+1}, \ldots, I_n\rangle$ and IE.

Proposition 1 [Soundness of the Box-Narrowing] Let $\langle c, i\rangle$ be a projection constraint, $\langle I_1, \ldots, I_n\rangle$ be a box, IE be a interval extension operator, and

$$\langle I_1,\ldots,I_{i-1},I,I_{i+1},\ldots,I_n\rangle = \texttt{BOX-NARROW}(\langle c,i\rangle,\langle I_1,\ldots,I_n\rangle,IE).$$

Then

$$r_1 \in I_1, \ldots, r_n \in I_n \;\&\; c(r_1,\ldots,r_n) \;\Rightarrow\; r_i \in I$$

Proof Assume that $r_1 \in I_1, \ldots, r_n \in I_n$ and that $r_i \notin I$. Then either $r_i < l_i$ or $r_i > u_i$, where $I_i = [l_i, u_i]$. If $r_i < l_i$, we have that

$$IE(c)(I_1,\ldots,I_{i-1},\overline{r_i},I_{i+1},\ldots,I_n)$$

by definition of an interval extension and

$$IE(c)(I_1,\ldots,I_{i-1},[u_i^-,u_i],I_{i+1},\ldots,I_n)$$

by hypothesis. Hence, c is box-consistent wrt $\langle I_1, \ldots, I_{i-1}, I \uplus \overline{r_i}, I_{i+1}, \ldots, I_n\rangle$ and IE, which contradicts our hypothesis that I is defined as the largest set included in I_i such that $\langle c, i\rangle$ is box-consistent with respect to $\langle I_1, \ldots, I_{i-1}, I, I_{i+1}, \ldots, I_n\rangle$ and IE. The case $r_i > u_i$ is similar. $\Box$

We are now in a position to define the pruning algorithm of `Newton` which consists essentially in applying the narrowing operators of each projection until no further reduction occurs. The pruning algorithm is depicted in Figure 1. It first applies box-consistency on the natural and distributed extensions until no further reduction occurs and then applies box-consistency on the Taylor extension. The two steps are iterated until a fixpoint is reached. Termination of the algorithm is guaranteed since the set $\mathcal{F}$ is finite and thus the intervals can only be reduced finitely often.

4.5 The Branch and Prune Algorithm `Newton`

Figure 2 is a very high level description of the branch and prune algorithm highlighting the control flow. The algorithm applies operation `PRUNE` on the initial box. If the resulting box is empty (which means that one of its components is empty), then there is no solution by Proposition 1. If the resulting box is small enough (specified by the desired accuracy in solutions), then it is included in the result. The function `BRANCH` splits the box into two subboxes along one dimension (variable). Variables for splitting are chosen by `BRANCH` using a round-robin heuristic.

5 Implementation of Box-Consistency

The purpose of this section is to show how to implement the narrowing operators for the various interval extensions. We start by describing a basic tool used in the implementations, then describe the various narrowing operators, and conclude by some implementation issues.

procedure PRUNE(**in** $\mathcal{S}$: Set of Constraint; **inout** $\vec{I}:\mathcal{I}^n$)
begin
    repeat
        $\vec{I_p}$:= $\vec{I}$;
        BOX-PRUNE($\mathcal{S}$,$\{NE, DE\}$,$\vec{I}$);
        BOX-PRUNE($cond(\mathcal{S},\vec{I})$,$\{TE(\vec{I})\}$,$\vec{I}$)
    until $\vec{I} = \vec{I_p}$;
end

procedure BOX-PRUNE(**in** $\mathcal{S}$: Set of Constraint; **in** SEO: Set of Operators; **inout** $\vec{I}:\mathcal{I}^n$)
begin
    repeat
        $\vec{I_p}$:= $\vec{I}$;
        $\vec{I}$:= $\bigcap\{$BOX-NARROW$((c,i),\vec{I},IE) \mid c \in \mathcal{S} \;\&\; 1 \le i \le n \;\&\; IE \in SEO\;\}$
    until $\vec{I} = \vec{I_p}$;
end

Figure 1: Pruning in Newton

procedure BranchAndPrune($\mathcal{S}$: Set of Constraint; $\vec{I_0}:\mathcal{I}^n$): Set of $\mathcal{I}^n$;
begin
  $\vec{I}$:= PRUNE($\mathcal{S}$,$\vec{I_0}$);
  if $\neg$ IsEmpty($\vec{I}$) **then**
    if IsSmallEnough($\vec{I}$) **then**
      return $\{\vec{I}\}$
    else
      $\langle\vec{I_1},\vec{I_2}\rangle$:= BRANCH($\vec{I}$);
      return BranchAndPrune($\mathcal{S}$,$\vec{I_1}$) $\cup$ BranchAndPrune($\mathcal{S}$,$\vec{I_2}$)
    endif
  else
    return $\emptyset$
  endif
end

Figure 2: The Branch and Prune Algorithm

```
function LNAR(F, F' : 𝓘 → 𝓘, I : 𝓘):  𝓘;
begin
    r := right(I);
    if 0 ∉ F(I) then
        return ∅;
    I := N*(F, F', I);
    if 0 ∈ F([left(I), left(I)+]) then
        return I ⊎ r̄
    else if
        ⟨I1, I2⟩ := SPLIT(I);
        if LNAR(F, F', I1) ≠ ∅ then
            return LNAR(F, F', I1) ⊎ r̄
        else
            return LNAR(F, F', I2) ⊎ r̄
    endif
end;
```

Figure 3: The function LNAR

5.1 Extreme Zeros of an Interval Function

Box-consistency can often be reduced to two subproblems which, informally speaking, consist in shrinking the left (resp. the right) of an interval I' to the leftmost (resp. rightmost) zero of a univariate interval function F in I'. The univariate interval function F is an extension of a real function f which is either univariate, in which case F is a traditional interval extension, or multivariate, in which case F is obtained by taking an interval extension of f and substituting all variables but one, say x_i, by their intervals. In addition, we will have at our disposal a function F', the "derivative" of F, which is either an interval extension of the derivative of f (univariate case) or an interval extension of the partial derivative of f wrt x_i in which all variables but x_i have been replaced by their intervals.

The subproblems can be computed using a variation of the univariate interval Newton method. The method uses the following property for pruning the search space

$$0 \in F(I) \;\Rightarrow\; 0 \in N(F, F', I)$$

where

$$N(F, F', I) = I \;\cap\; (\overline{center(I)} - \frac{F(\overline{center(I)})}{F'(I)}).$$

More precisely, the algorithm uses $N^*(F, F', I) = \bigcap_{i=0}^{\infty} I_i$ where

$$\begin{array}{lcl} I_0 & = & I \\ I_{i+1} & = & N(F, F', I_i) \;\; (0 \leq i) \end{array}$$

Figure 3 depicts a simple procedure LNAR to shrink to the leftmost zero (procedure RNAR is defined similarly). It make uses of a function SPLIT which, given an interval I, returns two intervals I_1 and

I_2 such that $I = I_1 \cup I_2$ and $\mathit{left}(I_2) = \mathit{right}(I_1)$. The algorithm first applies the pruning procedure. It terminates if the left zero has been found or the interval cannot contain a zero. Otherwise, the interval is split into two subintervals. The leftmost interval is explored first. If it does not contain a zero, the rightmost interval is explored.

5.2 Box-Consistency on the Natural Interval Extension

We are now in a position to define the narrowing operator for the natural interval extension. The basic idea is very simple. For a constraint $\langle f = 0, i\rangle$, it consists in taking an interval extension of F and replacing all variables but x_i by their interval I_i to obtain a univariate function. The leftmost and rightmost zeros are then computed to produce the result.

Definition 14 [Narrowing Operator for the Natural Interval Extension] The narrowing operator for the natural interval extension is defined as follows:

$\texttt{BOX-NARROW}(\langle f = 0, i\rangle, \langle I_1, \ldots, I_n\rangle, NE)$ = $\langle I_1, \ldots, I_{i-1}, I, I_{i+1}, \ldots, I_n\rangle$
where

$$\begin{array}{lll} I & = & \texttt{LNAR}(F, F', \texttt{RNAR}(F, F', I_i)) \\ F & = & \lambda X.\ NE(f)(I_1, \ldots, I_{i-1}, X, I_{i+1}, \ldots, I_n) \\ F' & = & \lambda X.\ DER(f, i)(I_1, \ldots, I_{i-1}, X, I_{i+1}, \ldots, I_n) \end{array}$$

It is important to note that box-consistency on the natural extension (and on the distributed extension as well) can be applied even if the function is not differentiable. It suffices to omit the application of operator N^* in the functions `LNAR` and `RNAR`.

5.3 Box-Consistency on the Distributed Interval Extension

We now turn to the narrowing operator for the distributed interval extension. Box-consistency on the distributed interval extension can be enforced by using the univariate interval function

$$F = \lambda X.\ DE(f)(I_1, \ldots, I_{i-1}, X, I_{i+1}, \ldots, I_n)$$

and by searching its extreme zeros. However, since the function is in distributed form, it is possible to do better by using an idea from [7]. The key insight is to sandwich F exactly between two univariate real functions f_l and f_u defined as follows:

$$\begin{array}{lll} f_l & = & \lambda x.\mathit{left}(F(\overline{x})) \\ f_u & = & \lambda x.\mathit{right}(F(\overline{x})). \end{array}$$

Box-consistency can now be enforced by searching the leftmost and rightmost zeros of some interval extensions, say F_l and F_u, of f_l and f_u using interval extensions, say F_l' and F_u', of their derivatives f_l' and f_u'. Of course, `LNAR` and `RNAR` can be used to find these extreme zeros.

The key advantage of the distributed interval extension is that it is easy to define the function f_l and f_u constructively. Let F be of the form

$$F = \lambda X.\ I_1 X^{n_1} + \ldots + I_p X^{n_p}.$$

Function f_l is defined as

$$f_l = \lambda x.\ \mathit{low}(I_1, x, n_1) + \ldots + \mathit{low}(I_p, x, n_p)$$

where

$$low(I,x,n) = \begin{cases} \mathit{left}(I)\ x^n & \text{if } x \geq 0 \vee j \text{ is even} \\ \mathit{right}(I)\ x^n & \text{otherwise} \end{cases}$$

Function f_u is defined as

$$f_u = \lambda x.\ \mathit{high}(I_1, x, n_1) + \ldots + \mathit{high}(I_p, x, n_p)$$

where

$$\mathit{high}(I,x,n) = \begin{cases} \mathit{right}(I)\ x^n & \text{if } x \geq 0 \vee j \text{ is even} \\ \mathit{left}(I)\ x^n & \text{otherwise} \end{cases}$$

It is easy to see that the two definitions of f_l and f_u are similar. The narrowing operator can now be obtained by using Newton interval method on the above two functions. Some care must be applied obviously since f_l and f_u are not differentiable at 0. The method is more efficient than applying the interval Newton method on the interval function, since intervals have been replaced by numbers increasing the precision of the Newton operator N^*. We now present the narrowing operator.

Definition 15 [Narrowing Operator for the Distributed Interval Extension] Let $\langle f = 0, i\rangle$ be a projection constraint, F be $\lambda X.\ DE(f)(I_1, \ldots, I_{i-1}, X, I_{i+1}, \ldots, I_n)$, f_l be $\lambda x.\mathit{left}(F(\overline{x}))$, f_u be $\lambda x.\mathit{right}(F(\overline{x}))$. Assuming that $\langle I_1, \ldots, I_n\rangle$ is not empty, the narrowing operator for the distributed interval extension is defined as follows:

$\texttt{BOX-NARROW}(\langle(f = 0, DE), i\rangle, \langle I_1, \ldots, I_n\rangle)$ = $\langle I_1, \ldots, I_{i-1}, [l_i, u_i], I_{i+1}, \ldots, I_n\rangle$
where

$$\begin{array}{lcl}
l_i & = & \begin{cases} l & \texttt{if } 0 \in F([l, l^+]) \\ \mathit{left}(\texttt{LNAR}(F_l, F_l', [l,0]) \cup \texttt{LNAR}(F_l, F_l', [0,u])) & \texttt{if } F([l, l^+]) \geq \overline{0} \\ \mathit{left}(\texttt{LNAR}(F_u, F_u', [l,0]) \cup \texttt{LNAR}(F_u, F_u', [0,u])) & \texttt{otherwise} \end{cases} \\
u_i & = & \begin{cases} u & \texttt{if } 0 \in F([u^-, u]) \\ \mathit{right}(\texttt{RNAR}(F_l, F_l', [l,0]) \cup \texttt{RNAR}(F_l, F_l', [0,u])) & \texttt{if } F([l, l^+]) \geq \overline{0} \\ \mathit{right}(\texttt{RNAR}(F_u, F_u', [l,0]) \cup \texttt{RNAR}(F_u, F_u', [0,u])) & \texttt{otherwise} \end{cases} \\
F_l & = & NE(f_l) \\
F_u & = & NE(f_u) \\
F_l' & = & DER(f_l) \\
F_u' & = & DER(f_u) \\
l & = & \mathit{left}(I_i) \\
u & = & \mathit{right}(I_i)
\end{array}$$

5.4 Taylor Interval Extension

We conclude by presenting the narrowing operator for the Taylor interval extension. Box-consistency on the Taylor interval extension can be enforced by using the interval function

$$F = \lambda X.\ TE(f, \langle I_1, \ldots, I_n\rangle)(I_1, \ldots, I_{i-1}, X, I_{i+1}, \ldots, I_n)$$

and by applying a simple implementation of LNAR and RNAR where the Newton operator N^* is omitted. However, it is possible to do better by noticing that the constraint is of the form

$$NE(f)(\overline{c_1},\ldots,\overline{c_n})+\sum_{j=1}^{i-1} DER(f,j)(\vec{I})(I_j-\overline{c_j})+DER(f,i)(I_1,\ldots,I_n)(X_i-\overline{c_i})+\sum_{j=i+1}^{n} DER(f,j)(\vec{I})(I_j-\overline{c_j}) = \overline{0}$$

where $c_i = center(I_i)$ and contains a single variable which can be isolated to compute box-consistency directly.

Definition 16 [Narrowing Operator for the Taylor Interval Extension] The narrowing operator for the Taylor interval extension is defined as follows:

$$\texttt{BOX-NARROW}(\langle f = 0, i\rangle, \langle I_1,\ldots,I_n\rangle, TE) = \langle I_1,\ldots,I_{i-1}, I, I_{i+1},\ldots,I_n\rangle$$

where

$$I = I_i \cap (\overline{c_i} - \frac{1}{DER(f,i)(I_1,\ldots,I_n)}[\sum_{j=1, j\neq i}^{n} DER(f,j)(I_1,\ldots,I_n)\,(I_j-\overline{c_j}) + NE(f)(\overline{c_1},\ldots,\overline{c_n})]).$$

and $c_i = center(I_i)$.

5.5 Implementation Issues

We now review some implementation issues which arise in programming the algorithm.

Priorities In the pruning algorithm, it is important for efficiency reasons to use a priority queue to ensure that projections over the distributed interval extension be selected before projections over the natural interval extension. Newton also does not enforce box-consistency on the distributed version whenever it is believed to lose too much precision (e.g. an expression raised to some power).

Precision In practice, it is often sufficient to return intervals whose widths[4] are within the desired accuracy instead of returning intervals of the form $[l, l^+]$. It is easy to modify the BRANCH operation to split only intervals whose widths is above the required accuracy. Our system allows users to specify the accuracy.

Improvement Factor Box-consistency can sometimes take much time to remove small parts of the intervals. In these cases, it is probably more cost-effective to branch. Once again, it is easy to modify the algorithm to avoid this problem by making sure that the narrowing operators do not update the intervals unless some significant reduction has taken place. Since the notion of significant reduction may be problem-dependent, our system lets users specify the improvement factor necessary to update an interval in a projection.

Automatic Differentiation As mentioned, our algorithm takes a very simple approach to obtain partial derivatives, i.e., no effort is spent in factoring common expressions to reduce the dependency problem of interval arithmetic. The main reason comes from the fact that we are using automatic differentiation [20] to evaluate the derivatives together with the functions. This choice may be reconsidered in a further version of the system.

[4] The width of $[l, u]$ is $u - l$.

Existence Proof of a Solution Box-consistency on a system of equations can be viewed as a generalization of Hansen-Segupta operator used in interval methods. This operator can be used to prove the existence of solutions. Our algorithm is organized to exploit this property so that it is able to report this information to users. See [9] for more discussion on this topic. No special effort was devoted to this topic however and it is certainly possible to do much better.

Inequalities It is simple to generalize the above algorithms for inequalities. In general, it suffices to test if the inequality is satisfied at the end points of the interval. If it is not, then the problem reduces once again to finding the leftmost and/or rightmost zeros.

6 Experimental Results

This section reports experimental results of `Newton` on a variety of standard benchmarks. The benchmarks were taken from papers on numerical analysis [16], interval analysis [5, 7, 15], and continuation methods [26, 18, 17, 11]. We also compare `Newton` with a traditional interval method using Hansen-Segupta's operator, range testing, and branching. This method uses the same implementation technology as `Newton` and is denoted by `HRB` in the following.[5] Finally, we compare `Newton` with a state-of-the-art continuation method [26], denoted by `CONT` in the following. Note that all results given in this section were obtained by running `Newton` on a `Sun Sparc 10` workstation to obtain all solutions. In addition, the final intervals must have widths smaller than 10^{-8} and `Newton` always uses an improvement factor of 10%. The results are summarized in Table 1. For each benchmark, we give the number of variables (n), the total degree of the system (d), the initial range for the variables, and the results of each method in seconds. Note that the times for the continuation method are on a `DEC 5000/200`. A space in a column means that the result is not available for the method. A question mark means that the method does not terminate in a reasonable time ($>$ 1 hour). The rest of the section describes each benchmark and the results in much more detail. For each benchmark, we report the CPU times in seconds, the growth of the CPU time, the number of branch operations *branching*, the number of narrowings on the various extensions *na-ne, na-ee, na-te*, the total number of narrowings *na-tot*, the number of function evaluations (including evaluation of derivatives) for each of the extensions *fe-ne, fe-ee, fe-te* and the total number of function evaluations *fe-tot*. We also indicate the number of preconditionings by *pr-con* and whether the algorithm can prove the existence of the solutions in the resulting intervals by *proof*.

6.1 Broyden Banded Functions

This is a traditional benchmark of interval techniques and was used for instance in [4]. It consists in finding the zeros of the functions

$$f_i(x_1,\ldots,x_n) = x_i(2+5x_i^2)+1-\textstyle\sum_{j\in J_i} x_j(1+x_j) \quad (1 \le i \le n)$$

where $J_i = \{j \mid j \neq i \ \& \ max(1, i-5) \le j \le min(n, i+1)\}$. One of the interesting features of this benchmark is that it is easy to scale up to an arbitrary dimension and hence provides a good

[5] Some interval methods such as [4] are more sophisticated than `HRB` but the sophistication aims at speeding up the computation near a solution. Our main contribution is completely orthogonal and aims at speeding up the computation when far from a solution and hence comparing it to `HRB` is meaningful.

Benchmarks	v	d	range	`Newton`	`HRB`	`CONT`
Broyden	10	3^{10}	[-1,1]	1.65	18.23	
Broyden	20	3^{20}	[-1,1]	4.25	?	
Broyden	320	3^{320}	[-1,1]	113.71	?	
Broyden	320	3^{320}	$[-10^8, 10^8]$	143.40	?	
Moré-Cosnard	20	3^{20}	$[-4, 5]$	24.49	968.25	
Moré-Cosnard	40	3^{40}	$[-4, 5]$	192.81	?	
Moré-Cosnard	80	3^{80}	$[-4, 5]$	1752.64	?	
Moré-Cosnard	80	3^{80}	$[-10^8, 0]$	1735.09	?	
i1	10	3^{10}	[-2,2]	0.06	14.28	
i2	20	3^{20}	[-1,2]	0.30	1821.23	
i3	20	3^{20}	[-2,2]	0.31	5640.80	
i4	10	6^{10}	[-1,1]	73.94	445.28	
i5	10	11^{10}	[-1,1]	0.08	33.58	
kin1	12	4608	$[-10^8, 10^8]$	14.24	1630.08	
kin2	8	256	$[-10^8, 10^8]$	353.06	4730.34	35.61
eco	4	18	$[-10^8, 10^8]$	0.60	2.44	1.13
eco	5	54	$[-10^8, 10^8]$	3.35	29.88	5.87
eco	6	162	$[-10^8, 10^8]$	22.53	?	50.18
eco	7	486	$[-10^8, 10^8]$	127.65	?	991.45
eco	8	1458	$[-10^8, 10^8]$	915.24	?	
eco	9	4374	$[-10^8, 10^8]$	8600.28	?	
combustion	10	96	$[-10^8, 10^8]$	9.94	?	57.40
chemistry	5	108	$[0, 10^8]$	6.32	?	56.55
neuro	6	1024	$[-10, 10]$	0.91	28.84	5.02
neuro	6	1024	$[-1000, 1000]$	172.71	?	5.02

Table 1: Summary of the Experimental Results

	5	10	20	40	80	160	320
CPU time	0.20	1.65	4.25	9.79	22.13	48.30	113.71
growth		8.25	2.57	2.30	2.26	2.18	2.35
branching	0	0	0	0	0	0	0
na-ne	57	260	661	1607	4351	8096	17126
na-ee	1226	8334	21236	48540	102797	206926	414798
na-te	35	110	260	560	1200	2400	4480
na-tot	1318	8704	22157	50707	108348	217422	436404
fe-ne	81	1828	2943	5103	11993	20431	42125
fe-ee	3462	21518	53722	121984	257398	517640	1036210
fe-te	95	320	920	2720	8800	30400	111360
fe-tot	3638	23666	57585	129807	278191	568471	1189695
pr-con	0	0	0	0	0	0	0
proof	yes	yes	yes	yes	yes	yes	yes

Table 2: `Newton` on the Broyden Banded functions with initial intervals $[-1, 1]$

	5	10	20	40	80	160	320
CPU time	0.31	2.15	5.09	12.49	27.69	61.60	143.40
growth		6.93	2.36	2.45	2.21	2.22	2.32
branching	0	0	0	0	0	0	0
pr-con	0	0	0	0	0	0	0
proof	yes	yes	yes	yes	yes	yes	yes

Table 3: `Newton` on the Broyden Banded functions with initial intervals $[-10^8, 10^8]$

basis to compare various methods. Table 2 reports the results of our algorithm for various sizes assuming initial intervals $[-1, 1]$.

The results indicate that `Newton` solves the problem using only constraint propagation: no branching is needed. In addition, the growth of the computation times is very low and indicates that `Newton` is essentially linear and can thus solve very large instances of this problem. Finally, `Newton` proves the existence of a solution in the final intervals. To our knowledge, no other algorithm has all these functionalities. Table 3 shows the same results when the initial intervals are $[-10^8, 10^8]$. They indicate that the CPU time increases only slightly in this problem when the initial intervals become substantially larger. It is interesting to note that substantial pruning is obtained by box-consistency on the natural and distributed extensions alone. For $n = 10$, maximal box-consistency on these two extensions produces the intervals

$$\begin{array}{l}
[-0.4283028737061274627, -0.4283028534683728794] \\
[-0.4765964317901201786, -0.4765964169224605195] \\
[-0.5196524683730758821, -0.5196524589206473754] \\
[-0.5580993358758108425, -0.5580993137885511545] \\
[-0.5925061654931400579, -0.5925061481657747375] \\
[-0.6245036923913307448, -0.6245036720076052594] \\
[-0.6232394806883442274, -0.6232394621928379896] \\
[-0.6213938520278742273, -0.6213938315652728361] \\
[-0.6204536054436834425, -0.6204535878744913413] \\
[-0.5864692773020701023, -0.5864692641387999616]
\end{array}$$

	5	10	20	40	80
CPU time	0.75	4.07	24.49	192.81	1752.64
growth		5.42	6.02	7.87	9.08
branching	0	0	0	0	0
na-ne	3663	12616	46555	213949	1236532
na-te	104	255	505	1005	2807
na-tot	3767	12871	47060	214954	1239339
fe-ne	8775	31837	107977	466595	2586907
fe-te	884	3111	11211	42411	166415
fe-tot	9659	34948	119188	509006	2753322
fe-grow		3.62	3.41	4.27	5.40
pr-con	1	1	1	1	1
proof	yes	no	no	no	no

Table 4: `Newton` on the Moré-Cosnard nonlinear integral Equation with initial intervals in $[-4, 5]$

which have widths lower than 10^{-6}. Note that the Hansen-Segupta's operator alone does not produce any pruning initially and returns the initial intervals whether they be of the form $[-10^8, +10^8]$ or $[-1, 1]$. This indicates that box-consistency on the natural and distributed interval extensions are particularly effective when far from a solution while box-consistency on the Taylor extension (and the Hansen-Segupta's operator) is effective when near a solution.

It is also interesting to stress the importance of box-consistency on the natural extension in this example to reduce the growth factor. Without it, the algorithm takes about 48 and 440 seconds instead of 27 and 61 for `Newton` for $n = 80$ and $n = 160$, since the distributed interval extension loses precision due to the dependency problem.

Finally, it is interesting to compare `Newton` with traditional interval methods. `HRB` takes 0.34 seconds on $n = 5$ with 18 branchings, about 18 seconds for $n = 10$ with about 300 branchings, and does not return after more than an hour on $n = 20$.

6.2 Discretization of a Nonlinear Integral Equation

This example comes from [16] and is also a standard benchmark for nonlinear equation solving . It consists in finding the root of the functions $f_k(x_1, \ldots, x_m)$ $(1 \leq k \leq m)$ defined as

$$x_k + \frac{1}{2(m+1)}[(1-t_k)\sum_{j=1}^{k} t_j(x_j + t_j + 1)^3 + t_k \sum_{j=k+1}^{m} (1-t_j)(x_j + t_j + 1)^3]$$

where $t_j = jh$ and $h = 1/(m+1)$. These functions come from the discretization of a nonlinear integral equation, giving a constraint system denser than the sparse constraint system for the Broyden banded functions. The variables x_i were given initial domains $[-4, 5]$ as in [21] and the computation results are given in Table 4.

Once again, it is interesting to note that `Newton` is completely deterministic on this problem, i.e. it does not do any branching. `Newton` is probably cubic in the number of variables for this problem. It is important to point out the critical role of box-consistency on the natural extension to solve this problem efficiently. `Newton` without the natural extension would not be deterministic and would slow down exponentially, since box-consistency on the distributed extension loses too

	5	10	20	40	80
CPU time	0.70	3.82	20.81	189.94	1735.09
growth		5.45	5.44	9.12	9.13
branching	0	0	0	0	0
pr-con	0	0	0	0	0
proof	yes	no	no	no	no

Table 5: `Newton` on the Moré-Cosnard nonlinear integral Equation with initial intervals in $[-10^8, 0]$

	5	10	20	40	80
CPU time	0.66	7.76	968.25	?	?
branching	5	24	508	?	?
fe-tot	3709	20194	1285764	?	?
pr-con	7	32	667	?	?
proof	yes	no	no	?	?

Table 6: The `HRB` algorithm on the Moré-Cosnard nonlinear integral Equation with initial intervals in $[-4, 5]$

much precision due to the dependency problem (multiple occurrences of the same variable) and box-consistency on the Taylor interval extension is not helpful initially. Once again, we observe that box-consistency over the natural extension is helpful when far from a solution while box-consistency on the Taylor extension is useful to terminate the search quickly. Table 5 gives the result for the initial intervals of size $[-10^8, 0]$, which shows that the algorithm continues to perform well in this case. Finally, Table 6 gives the results for the `HRB` algorithm on this problem. Once again, `Newton` outperforms the `HRB` method substantially.

6.3 Interval Arithmetic Benchmarks

This section considers standard benchmarks from interval arithmetic papers [14, 7]. Benchmark `i1` is the following set of equations

$$\left\{ \begin{array}{l}
0 = x_1 - 0.25428722 - 0.18324757\ x_4\ x_3\ x_9 \\
0 = x_2 - 0.37842197 - 0.16275449\ x_1\ x_{10}\ x_6 \\
0 = x_3 - 0.27162577 - 0.16955071\ x_1\ x_2\ x_{10} \\
0 = x_4 - 0.19807914 - 0.15585316\ x_7\ x_1\ x_6 \\
0 = x_5 - 0.44166728 - 0.19950920\ x_7\ x_6\ x_3 \\
0 = x_6 - 0.14654113 - 0.18922793\ x_8\ x_5\ x_{10} \\
0 = x_7 - 0.42937161 - 0.21180486\ x_2\ x_5\ x_8 \\
0 = x_8 - 0.07056438 - 0.17081208\ x_1\ x_7\ x_6 \\
0 = x_9 - 0.34504906 - 0.19612740\ x_{10}\ x_6\ x_8 \\
0 = x_{10} - 0.42651102 - 0.21466544\ x_4\ x_8\ x_1
\end{array} \right.$$

with initial intervals $[-2,2]$. Benchmark `i2` is the set of equations

$$\begin{cases} 0 = x_1 - 0.24863995 - 0.19594124\, x_7\, x_{10}\, x_{16} \\ 0 = x_2 - 0.87528587 - 0.05612619\, x_{18}\, x_8\, x_{11} \\ 0 = x_3 - 0.23939835 - 0.20177810\, x_{10}\, x_7\, x_{11} \\ 0 = x_4 - 0.47620128 - 0.16497518\, x_{12}\, x_{15}\, x_1 \\ 0 = x_5 - 0.24711044 - 0.20198178\, x_8\, x_9\, x_{16} \\ 0 = x_6 - 0.33565227 - 0.15724045\, x_{16}\, x_{18}\, x_{11} \\ 0 = x_7 - 0.13128974 - 0.12384342\, x_{12}\, x_{13}\, x_{15} \\ 0 = x_8 - 0.45937304 - 0.18180253\, x_{19}\, x_{15}\, x_{18} \\ 0 = x_9 - 0.46896600 - 0.21241045\, x_{13}\, x_2\, x_{17} \\ 0 = x_{10} - 0.57596835 - 0.16522613\, x_{12}\, x_9\, x_{13} \\ 0 = x_{11} - 0.56896263 - 0.17221383\, x_{16}\, x_{17}\, x_8 \\ 0 = x_{12} - 0.70561396 - 0.23556251\, x_{14}\, x_{11}\, x_4 \\ 0 = x_{13} - 0.59642512 - 0.24475135\, x_7\, x_{16}\, x_{20} \\ 0 = x_{14} - 0.46588640 - 0.21790395\, x_{13}\, x_3\, x_{10} \\ 0 = x_{15} - 0.10607114 - 0.20920602\, x_1\, x_9\, x_{10} \\ 0 = x_{16} - 0.26516898 - 0.21037773\, x_4\, x_{19}\, x_9 \\ 0 = x_{17} - 0.20436664 - 0.19838792\, x_{20}\, x_{10}\, x_{13} \\ 0 = x_{18} - 0.56003141 - 0.18114505\, x_6\, x_{13}\, x_8 \\ 0 = x_{19} - 0.92894617 - 0.04417537\, x_7\, x_{13}\, x_{16} \\ 0 = x_{20} - 0.57001682 - 0.17949149\, x_1\, x_3\, x_{11} \end{cases}$$

with initial intervals $[-1,2]$. Benchmark `i3` has the same set of equations as `i2` but has initial intervals $[-2,2]$. Benchmark `i4` has the set of equations

$$\begin{cases} 0 = x_1^2 - 0.25428722 - 0.18324757\, x_4^2\, x_3^2\, x_9^2 \\ 0 = x_2^2 - 0.37842197 - 0.16275449\, x_1^2\, x_{10}^2\, x_6^2 \\ 0 = x_3^2 - 0.27162577 - 0.16955071\, x_1^2\, x_2^2\, x_{10}^2 \\ 0 = x_4^2 - 0.19807914 - 0.15585316\, x_7^2\, x_1^2\, x_6^2 \\ 0 = x_5^2 - 0.44166728 - 0.19950920\, x_7^2\, x_6^2\, x_3^2 \\ 0 = x_6^2 - 0.14654113 - 0.18922793\, x_8^2\, x_5^2\, x_{10}^2 \\ 0 = x_7^2 - 0.42937161 - 0.21180486\, x_2^2\, x_5^2\, x_8^2 \\ 0 = x_8^2 - 0.07056438 - 0.17081208\, x_1^2\, x_7^2\, x_6^2 \\ 0 = x_9^2 - 0.34504906 - 0.19612740\, x_{10}^2\, x_6^2\, x_8^2 \\ 0 = x_{10}^2 - 0.42651102 - 0.21466544\, x_4^2\, x_8^2\, x_1^2 \end{cases}$$

and initial intervals $[-1,1]$. The number of solutions must be a multiple of 1024. Benchmark `i5` has the following set of equations

$$\begin{cases} 0 = x_1 - 0.25428722 - 0.18324757\, x_4^3\, x_3^3\, x_9^3 + x_3^4\, x_9^7 \\ 0 = x_2 - 0.37842197 - 0.16275449\, x_1^3\, x_{10}^3\, x_6^3 + x_{10}^4\, x_6^7 \\ 0 = x_3 - 0.27162577 - 0.16955071\, x_1^3\, x_2^3\, x_{10}^3 + x_2^4\, x_{10}^7 \\ 0 = x_4 - 0.19807914 - 0.15585316\, x_7^3\, x_1^3\, x_6^3 + x_1^4\, x_6^7 \\ 0 = x_5 - 0.44166728 - 0.19950920\, x_7^3\, x_6^3\, x_3^3 + x_6^4\, x_3^7 \\ 0 = x_6 - 0.14654113 - 0.18922793\, x_8^3\, x_5^3\, x_{10}^3 + x_5^4\, x_{10}^7 \\ 0 = x_7 - 0.42937161 - 0.21180486\, x_2^3\, x_5^3\, x_8^3 + x_5^4\, x_8^7 \\ 0 = x_8 - 0.07056438 - 0.17081208\, x_1^3\, x_7^3\, x_6^3 + x_7^4\, x_6^7 \\ 0 = x_9 - 0.34504906 - 0.19612740\, x_{10}^3\, x_6^3\, x_8^3 + x_6^4\, x_8^7 \\ 0 = x_{10} - 0.42651102 - 0.21466544\, x_4^3\, x_8^3\, x_1^3 + x_8^4\, x_1^7 \end{cases}$$

	i1	i2	i3	i4	i5
CPU time	0.06	0.30	0.31	73.94	0.08
branching	0	0	0	1023	0
na-ee	625	2107	1949	290776	381
na-te	0	80	80	37930	21
na-tot	625	2187	2029	328706	401
fe-ee	1760	5698	5318	752220	992
fe-te	0	560	560	269760	140
fe-tot	1760	6258	5878	1021980	1132
pr-con	0	1	1	1939	1
proof	yes	yes	yes	yes	yes

Table 7: `Newton` on the Traditional Interval Arithmetic Benchmarks

	i1	i2	i3	i4	i5
CPU time	14.28	1821.23	5640.80	445.28	33.58
branching	498	9031	36933	11263	1173
fe-tot	77380	6441640	19979025	2554066	154948
pr-con	586	12817	42193	14335	1211
proof	yes	yes	yes	yes	yes

Table 8: `HRB` on the Traditional Interval Arithmetic Benchmarks

and initial intervals $[-1, 1]$.

`Newton` solves all the problems with one solution without branching and solves the problem having 1024 solutions with 1023 branchings. Note also that box-consistency on the distributed extension solves benchmark `i1` alone. The results once again confirm our observation on when the various extensions are useful. Closely related results were observed in [7] on these benchmarks (see the related work section for a more detailed comparison) but our algorithm is in general about 4 times faster (assuming similar machines) and does not do any branching on `i5`. Table 8 also describes the results for the traditional interval arithmetic method. The importance of box-consistency on the distributed extension can easily be seen from these results. Note also that `Newton` (and interval methods) can prove the existence of a solution in the final intervals for all these problems.

It is also interesting to note that problem `i4` can be solved dramatically more efficiently simply by introducing intermediary variables $y_i = x_i^2$. The excution times then dropped to less than 0.5 seconds.

6.4 Kinematics Applications

We now describe the performance of `Newton` on two kinematics examples. Application `kin1` comes from robotics and describes the inverse kinematics of an elbow manipulator [7]. It consists of a

- 0.249150680	+ 0.125016350	- 0.635550070	+ 1.48947730
+ 1.609135400	- 0.686607360	- 0.115719920	+ 0.23062341
+ 0.279423430	- 0.119228120	- 0.666404480	+ 1.32810730
+ 1.434801600	- 0.719940470	+ 0.110362110	- 0.25864503
+ 0.000000000	- 0.432419270	+ 0.290702030	+ 1.16517200
+ 0.400263840	+ 0.000000000	+ 1.258776700	- 0.26908494
- 0.800527680	+ 0.000000000	- 0.629388360	+ 0.53816987
+ 0.000000000	- 0.864838550	+ 0.581404060	+ 0.58258598
+ 0.074052388	- 0.037157270	+ 0.195946620	- 0.20816985
- 0.083050031	+ 0.035436896	- 1.228034200	+ 2.68683200
- 0.386159610	+ 0.085383482	+ 0.000000000	- 0.69910317
- 0.755266030	+ 0.000000000	- 0.079034221	+ 0.35744413
+ 0.504201680	- 0.039251967	+ 0.026387877	+ 1.24991170
- 1.091628700	+ 0.000000000	- 0.057131430	+ 1.46773600
+ 0.000000000	- 0.432419270	- 1.162808100	+ 1.16517200
+ 0.049207290	+ 0.000000000	+ 1.258776700	+ 1.07633970
+ 0.049207290	+ 0.013873010	+ 2.162575000	- 0.69686809

Table 9: Coefficients for the Inverse Kinematics Example.

sparse system with 12 variables and the set of equations is as follows:

$$\begin{cases} s_2c_5s_6 - s_3c_5s_6 - s_4c_5s_6 + c_2c_6 + c_3c_6 + c_4c_6 = 0.4077 \\ c_1c_2s_5 + c_1c_3s_5 + c_1c_4s_5 + s_1c_5 = 1.9115 \\ s_2s_5 + s_3s_5 + s_4s_5 = 1.9791 \\ c_1c_2 + c_1c_3 + c_1c_4 + c_1c_2 + c_1c_3 + c_1c_2 = 4.0616 \\ s_1c_2 + s_1c_3 + s_1c_4 + s_1c_2 + s_1c_3 + s_1c_2 = 1.7172 \\ s_2 + s_3 + s_4 + s_2 + s_3 + s_2 = 3.9701 \\ s_i^2 + c_i^2 = 1 \qquad (1 \leq i \leq 6). \end{cases}$$

The second benchmark, denoted by `kin2`, is from [17] and describes the inverse position problem for a six-revolute-joint problem in mechanics. The equations which describe a denser constraint system are as follows:

$$\begin{cases} x_i^2 + x_{i+1}^2 - 1 = 0 \quad (1 \leq i \leq 4) \\ a_{1i}x_1x_3 + a_{2i}x_1x_4 + a_{3i}x_2x_3 + a_{4i}x_2x_4 + a_{5i}x_5x_7 + a_{6i}x_5x_8 + a_{7i}x_6x_7 + a_{8i}x_6x_8 \\ a_{9i}x_1 + a_{10i}x_2 + a_{11i}x_3 + a_{12i}x_4 + a_{13i}x_5a_{14i}x_6 + a_{15i}x_7 + a_{16i}x_8 + a_{17i} = 0 \;\; (1 \leq i \leq 4) \end{cases}$$

where the coefficients a_{ki} are given in table 9. In both examples, the initial intervals were given as $[-10^8, 10^8]$.

The results of `Newton` on these two benchmarks are given in Table 10. `Newton` is fast on the first benchmark and does not branch much to obtain all solutions. The algorithm in [7] branches more (the reported figure is 257 branches but it is not really comparable due to the nature of the algorithm) and is about 16 times slower on comparable machines. We are not aware of the results of continuation methods on this problem. `Newton` is slower on the second application and takes about 6 minutes. The continuation method described in [26] requires about 30 seconds on a `DEC 5000/200`. This method exploits the fact that the Newton polytopes for the last 4 equations are the same. Note that `HRB` requires about 1630 and 4730 seconds on these examples. Note also that

	`kin1`	`kin2`
CPU time	14.240	353.06
branching	89	5693
na-ee	17090	784687
na-te	10176	123032
na-tot	27266	907719
fe-ee	45656	1714779
fe-te	62080	854384
fe-tot	107736	2569163
pr-con	163	9505
proof	yes	yes

Table 10: `Newton` on the Kinematics Benchmarks

	4	5	6	7	8	9
CPU time	0.21	1.22	8.20	46.59	352.80	3311.42
growth		5.80	6.72	5.68	7.57	9.38
branching	24	119	517	2231	12248	82579
na-ee	834	4701	42481	214430	1622417	14031838
na-te	480	1976	6325	29238	157402	1219960
na-tot	1314	6677	48806	243668	1779819	15251798
fe-ee	2220	116628	99994	489894	3626847	30782836
fe-te	1293	6304	29825	160284	1062789	9118448
fe-tot	3513	17932	129819	650178	4689636	39901284
pr-con	37	147	687	2828	15265	104352
proof	yes	yes	yes	yes	yes	yes

Table 11: `Newton` on the economics modelling problem with initial intervals in $[-100, 100]$

`Newton` can prove the existence of solutions in the final intervals for these problems and that our computer representation uses intermediate variables

$$\begin{cases} x_{13} = x_4 + x_6 + x_8 \\ x_{14} = x_3 + x_5 + x_7 \\ x_{15} = x_4 + x_6 + x_8 \\ x_{16} = 3 * x_4 + 2 * x_6 + x_8 \end{cases}$$

to improve efficiently slightly in the first problem.

6.5 An Economics Modelling Application

The following example is taken from [18]. It is a difficult economic modelling problem that can be scaled up to arbitrary dimensions. For a given dimension n, the problem can be stated as the system

$$\begin{cases} (x_k + \sum_{i=1}^{n-k-1} x_i x_{i+k}) x_n - c_k = 0 \quad (1 \le k \le n-1) \\ \sum_{l=1}^{n-1} x_l + 1 = 0 \end{cases}$$

and the constants can be chosen at random.

Table 11 reports the results for various values of n with an initial interval of $[-100, 100]$. It is interesting to compare those results with the continuation methods presented in [26]. [26] reports

	4	5	6	7	8	9
CPU time	0.60	3.35	22.53	127.65	915.24	8600.28
growth		5.58	6.72	5.66	7.16	9.39
branching	102	500	1778	7527	38638	244263
na-ee	2689	15227	122662	606805	4413150	36325819
na-te	978	3296	14055	64632	366436	2647016
na-tot	3667	18523	136717	671437	4779586	38972835
fe-ee	7140	38160	291206	1400216	9913850	80264897
fe-te	3288	15024	80110	429396	2825368	22672208
fe-tot	10428	53184	371716	1829612	12739218	102937105
pr-con	148	527	2080	8337	42704	271534
proof	yes	yes	yes	yes	yes	yes

Table 12: `Newton` on the economics modelling problem with initial intervals in $[-10^8, 10^8]$

times (on a DEC-5000/200) of about 1 second for $n = 4$, 6 seconds for $n = 5$, 50 seconds for $n = 6$ and 990 seconds for $n = 7$. `Newton` is substantially faster on this problem than this continuation method, since it takes about 47 seconds for $n = 7$. More importantly, the growth factor seems much lower in `Newton`. The continuation method has growths of about 8 and 20 when going from 5 to 6 and 6 to 7, while `Newton` has growths of about 6.72 and 5.68. Table 12 gives the same results for initial intervals in $[-10^8, 10^8]$. It is interesting to note that the computation times increase by less than a factor 3 and that the growth factor is independent of the initial intervals. Note also that Newton can establish the existence of solutions for these problems. Finally, it is worthwhile stating that the results were obtained for a computer representation where x_n has been eliminated in a problem of dimension n.

6.6 Combustion Application

This problem is also from Morgan's book [18] and represents a combustion problem for a tempara-ture of 3000°. The problem is described by the following sparse systems of equations

$$\left\{\begin{array}{l} x_2 + 2\ x_6 + x_9 + 2\ x_{10} = 10^{-5} \\ x_3 + x_8 = 3\ 10^{-5} \\ x_1 + x_3 + 2\ x_5 + 2\ x_8 + x_9 + x_{10} = 5\ 10^{-5} \\ x_4 + 2\ x_7 = 10^{-5} \\ 0.5140437\ 10^{-7}\ x_5 = x_1^2 \\ 0.1006932\ 10^{-6}\ x_6 = 2\ x_2^2 \\ 0.7816278\ 10^{-15}\ x_7 = x_4^2 \\ 0.1496236\ 10^{-6}\ x_8 = x_1\ x_3 \\ 0.6194411\ 10^{-7}\ x_9 = x_1\ x_2 \\ 0.2089296\ 10^{-14}\ x_{10} = x_1\ x_2^2 \end{array}\right.$$

which is typical of chemical equilibrium systems. Table 13 describes the results of `Newton` on for the initial intervals $[-1, 1]$ and $[-10^8, 10^8]$. `Newton` behaves well on this example, since the continuation method of [26] takes about 57 seconds. Note once again that a substantial increase in the size of the initial intervals only induces a slowdown of about 2.5 for `Newton`. Note also that `Newton` can prove the existence of the solutions and that we use a formulation where variable x_7 and x_3 have been eliminated.

	[-1,1]	[-10^8,10^8]
CPU time	4.06	9.94
branching	183	523
na-ee	10676	28473
na-te	5248	7952
na-tot	15924	36425
fe-ee	28928	77508
fe-te	22464	49632
fe-tot	51392	127140
pr-con	187	527
proof	yes	yes

Table 13: `Newton` on the Combustion Problem.

CPU time	*branching*	*na-ee*	*na-te*	*na-tot*	*fe-ee*	*fe-te*	*fe-tot*	*pr-con*	*proof*
6.32	256	13725	3400	17125	34811	17425	52236	425	yes

Table 14: `Newton` on the Chemestry Problem with Initial Intervals $[0, 10^8]$

6.7 Chemical Equilibrium Application

This problem originates from [11] and describes a chemical equilibrium system. The set of equations is as follows:

$$
\begin{cases}
R = 10 \\
R_5 = 0.193 \\
R_6 = 0.002597/\sqrt{40} \\
R_7 = 0.003448/\sqrt{40} \\
R_8 = 0.00001799/40 \\
R_9 = 0.0002155/\sqrt{40} \\
R_{10} = 0.00003846/40 \\
x_1\ x_2 + x_1 - 3\ x_5 = 0 \\
2\ x_1\ x_2 + x_1 + x_2\ x_3^2 + R_8\ x_2 - R\ x_5 + 2\ R_{10}\ x_2^2 + R_7\ x_2\ x_3 + R_9\ x_2\ x_4 = 0 \\
2\ x_2\ x_3^2 + 2\ R_5\ x_3^2 - 8\ x_5 + R_6\ x_3 + R_7\ x_2\ x_3 = 0 \\
R_9\ x_2\ x_4 + 2\ x_4^2 - 4\ R\ x_5 = 0 \\
x_1\ x_2 + x_1 + R_{10}\ x_2^2 + x_2\ x_3^2 + R_8\ x_2 + R_5\ x_3^2 + x_4^2 - 1 + R_6\ x_3 + R_7\ x_2\ x_3 + R_9\ x_2\ x_4 = 0
\end{cases}
$$

and all x_i's must be positive. The results are depicted in Table 14 for an initial interval $[0, 10^8]$. They indicate that `Newton` is particularly effective on this problem, since it takes about 6 seconds and proves the existence of a solution in the final intervals. Note that the continuation method of [26] takes about 56 seconds on this problem.

	$[-10, 10]$	$[-10^2, 10^2]$	$[-10^3, 10^3]$	$[-10^4, 10^4]$
CPU time	0.91	11.69	172.71	2007.51
growth		12.84	14.77	11.62
branching	52	663	9632	115377
na-ee	4290	57224	645951	6541038
na-te	810	6708	96888	1173456
na-tot	5100	63932	742839	7714494
fe-ee	11012	144843	1620538	16647442
fe-te	4104	48804	769056	9376632
fe-tot	15116	193647	2389594	26024074
pr-con	69	983	15980	195270
proof	yes	yes	yes	yes

Table 15: `Newton` on the Neurophysiology Problem.

6.8 A Neurophysiology Application

We conclude the experimental section by showing an example illustrating the limitations of `Newton`. The application is from neurophysiology [26] and consists of the following system of equations:

$$\begin{cases} x_1^2 + x_3^2 = 1 \\ x_2^2 + x_4^2 = 1 \\ x_5\ x_3^3 + x_6\ x_4^3 = c_1 \\ x_5\ x_1^3 + x_6\ x_2^3 = c_2 \\ x_5\ x_1\ x_3^2 + x_6\ x_4^2\ x_2 = c_3 \\ x_5\ x_1^2\ x_3 + x_6\ x_2^2\ x_4 = c_4 \end{cases}$$

No initial intervals for the variables were given and the constants c_i can be chosen at random. The continuation method of [26] solves this problem in about 6 seconds. The results of `Newton` are depicted in Table 15 for various initial intervals. `Newton` is fast when the initial intervals are small (i.e., $[-10, 10]$). Unfortunately, the running time of the algorithm increases linearly with the size of the initial intervals, showing a limitation of the method on this example.

7 Related Work and Discussion

The research described in this paper originated in an attempt to improve the efficiency of constraint logic programming languages based on intervals such as `BNR-Prolog` [19] and `CLP(BNR)` [3]. These Constraint Logic Programming languages use constraint solving as basic operation and they were based on the simple generalization of arc-consistency described previously, i.e.

$$I_i = box\{I_i \cap \{\ r_i \ \mid\ \exists r_1 \in I_1, \ldots, \exists r_{i-1} \in I_{i-1}, \ldots, \exists r_{i+1} \in I_{i+1}, \ldots, \exists r_n \in I_n : c(r_1, \ldots, r_n)\ \}\}.$$

This approximation was enforced on simple constraints such as

$$x_1 = x_2 + x_3, \quad x_1 = x_2 - x_3, \quad x_1 = x_2 \times x_3$$

and complex constraints were decomposed in terms of these simple constraints.

As mentioned earlier, this approach is not very effective [2] and our main goal was to design new approximations of arc-consistency that could make use of existing interval methods. The main problem was the difficulty in characterizing the pruning of the Newton operator N^* in a declarative way (in order to introduce it nicely in the above programming languages) and box-consistency emerged as an attempt to generalize the operator to make sure that the bounds of the interval were locally consistent. Subsequent research made us realize that box-consistency is independent of the Newton operator and can be enforced even if the functions are not continuous or differentiable. In addition, the value of applying box-consistency on several extensions became clear. On the one hand, box-consistency on the Taylor extension generalizes interval methods based on Gauss-Seidel iterations and enables us to capture nicely Hansen-Segupta's operator. On the other hand, box-consistency on the natural and distributed extensions is really orthogonal to the pruning obtained from the Taylor expansion, producing a particularly effective algorithm. It is also worth pointing out that `Newton` spends most time in the natural and distributed extensions. However, for many applications, the use of the Taylor interval extension is critical to terminate the search quickly and to avoid generating many small intervals around the solutions. As a general observation, box-consistency on the natural and distributed extensions seem effective when far from a solution while box-consistency on the Taylor expansion seems effective when near a solution. It is worth mentioning that that the interval community has spent much effort to design additional techniques to speed up further the computation when near a solution but have not considered techniques to improve pruning when far from a solution.

It is interesting to note that the idea of using approximations of arc-consistency was also used independently by Hong and Stahl [7], who were also exposed to research on Constraint Logic Programming. Their use of projections is however quite different from ours. The key idea is to work with a set of boxes and to use projections to split a box into several subboxes by isolating all zeros of a projection. This gives an algorithm of a very different nature which cannot easily be characterized as a branch & prune algorithm since constraints are used to branch. Our approach seems to be more effective in practice, since their use of projections may generate many subboxes that may all need to be pruned away later on, implying much redundant work. Our approach postpones the branching until no pruning takes place and generates only subboxes when they are strictly necessary to progress. It is also very interesting to report that, on all benchmarks that we tested, the projection never contained more than two zeros. This seems to indicate that searching for all zeros may not be worthwhile in most cases and that box-consistency may be the right trade-off here. Finally, note that their approach seems to use implicitly an distributed extension[6] but they do not make use of the natural extension which is very important for some applications.

The research described here also provides a uniform framework to integrate these techniques in Constraint Logic Programming, to understand the importance of the various pruning operators and their relationships and to suggest further research directions. For instance, higher notions of consistency such as path-consistency [12] may be worth investigating for some applications.

8 Conclusion

In this paper, we presented a branch & prune algorithm to find all isolated solutions to a system of polynomial constraints over the reals. The algorithm is based on a single concept, box-consistency,

[6] The idea of sandwitching the interval function in between two real functions is described there.

which is an approximation of arc-consistency, a notion well-known in artificial intelligence. Box-consistency can be instantiated to produce Hansen-Segupta operator as well as other narrowing operators which are more effective when the computation is far from a solution. The algorithm and its mathematical foundations are simple. Moreover, the algorithm is shown to behave well on a variety of benchmarks from kinematics, mechanics, chemistry, combustion, and economics. It outperforms the interval methods we know of and compares well with continuation methods on their benchmarks. In addition, problems such as the Broyden banded function and the Moré-Cosnard discretization of a nonlinear integral equation can be solved for several hundred variables. Limitations of the method (e.g. a sensitivity to the size of the initial intervals on some problems) have also been identified.

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