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Abstract: We describe here the package subdivision_solver for the mathematical software SageMath. It provides a solver on real numbers for square systems of large dense polynomials. By large polynomials we mean multivariate polynomials with large degrees, which coefficients have large bit-size. While staying robust, symbolic approaches to solve systems of polynomials see their performances dramatically affected by high degree and bit-size of input polynomials. Available numeric approaches suffer from the cost of the evaluation of large polynomials and their derivatives. Our solver is based on interval analysis and bisections of an initial compact domain of \mathbb{R}^n where solutions are sought. Evaluations on intervals with Horner scheme is performed by the package fast_polynomial for SageMath. The non-existence of a solution within a box is certified by an evaluation scheme that uses a Taylor expansion at order 2, and existence and uniqueness of a solution within a box is certified with krawczyk operator. The precision of the working arithmetic is adapted on the fly during the subdivision process and we present a new heuristic criterion to decide if the arithmetic precision has to be increased.

Key-words: Interval Arithmetic, Subdivision, Adaptive Multi-Precision, Real Solutions, Large Dense Polynomials

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Un solveur par subdivision pour des systèmes de polynômes denses de haut degré et grande bit-size

Résumé: Le présent rapport décrit le package subdivision_solver pour SageMath, dédié à la résolution réelle de systèmes bien posés (i.e. avec autant d'équations que d'inconnues) dont les équations sont des polynômes denses de haut degrés et grande bit-size. Les approches de résolution symboliques et numériques voient leur performances très affectées par l'augmentation du degré et de la bit-size des polynômes. Les premières en raison du calcul exact sur des grands nombres, les secondes à cause du coût des évaluations des fonctions et de leur dérivées. Le solveur décrit ici est basé sur l'arithmétique par intervalles et s'appuie sur le package fast_polynomial pour SageMath qui permet l'évaluation rapide de polynômes sur des intervalles grâce entre autres au schéma de Horner. Les solutions sont cherchées dans un domaine initial compact de \mathbb{R}^n qui est subdivisé jusqu'à pouvoir soit prouver l'absence de solutions grâce à un développement de Taylor à l'ordre 2 soit prouver l'existence et l'unicité d'une solution en utilisant l'opérateur de Krawczyk. La précision arithmétique avec laquelle les calculs sont réalisés est adaptée pendant la résolution. On présente un nouveau critère, utilisé comme heuristique, pour décider s'il est nécessaire d'accroître la précision.

Mots-clés: Arithmétique par intervalles, subdivision, précision multiple adaptative, solutions réelles, polynômes denses de haut degré et grande bit-size

1 Introduction

subdivision_solver is a solver for square systems of polynomial equations using exhaustive search in an initial bounded real domain given as a box (i.e. a vector of intervals). It is specifically designed to handle systems of large dense polynomials and uses adaptive multiprecision arithmetic to stay robust to hard cases. subdivision_solver is proposed as a package for the mathematical software SageMath¹. It is based on the package fast_polynomial (see [5]) for SageMath that provides fast evaluation of polynomials on intervals and uses Horner forms.

The strategies that underlies the design of subdivision_solver are:

- using as much as possible double precision interval arithmetic: in this case interval computations are supported by the boost² interval library that is efficient. When the arithmetic precision is increased, interval computations are supported by the Multi-Precision Floating-point Interval library mpfi (see [8]) that allows arbitrary arithmetic precision.
- using partial derivatives at second order to obtain sharp interval evaluations; partial derivatives are symbolically computed at the initialization of the solving.
- minimizing evaluations of polynomials and their derivatives that are costly.

The rest of this report is organized as follows. Sec. 2 gives some basics on interval analysis and describes the main tools the solver uses. Sec. 3 presents three criteria that are used to decide to increase arithmetic precision. The two first come from the state of the art, the third is new. Sec. 4 describes the algorithms that we implemented. Sec. 5 proposes some numerical results. The rest of the introduction overviews installation and usage of the package.

A short user manual

subdivision_solver is a package for SageMath, and works with versions newer than 7.0. Its sole dependency is the package fast_polynomial³ for SageMath that provides fast evaluation of polynomials on intervals and uses Horner forms. After it has been download, move to the directory where it is and install it with sage fast_polynomial-0.9.4.spkg. Then download subdivision_solver⁴ and install it with the command sage subdivision_solver-0.0.1.spkg. Thats it.

We give here an example of use of subdivision_solver on randomly generated polynomials.

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Above instructions can be either copy-pasted in a sage console to be executed, or copy pasted in a file myfile.sage and executed with the command sage myfile.sage.

The initializer of the class subdivision_solver takes as arguments a list of polynomial and the list of variables of the polynomial ring.

The method solve takes as first argument the domain where the real solutions are sought, written as a column vector of RealIntervalField elements. Notice that the arithmetic precision of the first element of the domain determines the initial precision. The arithmetic precision is at least 53. When it is 53, bounds and intervals are double precision floating points, and operations on intervals are directly transposed into operations on double with boost.

To solve the system given as input, the initial domain will be subdivided and/or contracted into sub-domains; the second argument of the method solve is the minimum width of sub-domains to be explored during the resolution. It can be zero, and in this case the process is not guaranteed to terminate, in particular if the system admits a root with multiplicity.

When solving the system given in input, it can arise that arithmetic precision is not sufficient when, for instance, subdividing a box does not help to decide where is a solution due to accumulation of errors in interval computations. Such cases are detected, and the arithmetic precision is increased to face it. The third argument of solve is an upper bound of the arithmetic precision used to compute with intervals. Precision can be arbitrary large. mpfi is used when the precision is larger than 53.

The last argument of the method solve is a string determining whether statistics of the process are printed or not. Its value can be in { 'silent', 'stats', 'stats_color' }.

The output of solve is an integer with the following meaning:

- 0 Each solution lying in the interior of the initial domain has bean isolated in a box; isolating boxes of solutions are obtained with getSolutions.
- 1 Only a subset of solutions have been isolated; boxes that may contain solutions are obtained with getUndetermined but exploring these boxes will require a larger arithmetic precision than initially allowed.
- 2 Only a subset of solutions have been isolated; boxes of width smaller than allowed and/or requiring larger arithmetic precision where encountered.

Finally, giving a real number **r** as argument to the method **getSolutions** makes width of boxes isolating solutions that are returned smaller than **r** if maximum precision allows it. Otherwise isolating boxes will have width as small as possible.

2 Some tools of Interval Analysis

2.1 Notations

Let \mathbb{IR} be the set of non-empty closed interval of \mathbb{R} . We will denote an element of \mathbb{IR} with a lowercase bold letter as \mathbf{x} . If $\mathbf{x} \in \mathbb{IR}$, we will denote by $l(\mathbf{x})$ (resp. $u(\mathbf{x})$) its lower (resp. upper) bound, by $w(\mathbf{x})$ its width defined as $u(\mathbf{x}) - l(\mathbf{x})$ and by $m(\mathbf{x})$ its center (that is $l(\mathbf{x}) + \frac{w(\mathbf{x})}{2}$). The interior $|l(\mathbf{x}), u(\mathbf{x})|$ of \mathbf{x} will be denoted by $int(\mathbf{x})$ and its boundary $\mathbf{x} \setminus int(\mathbf{x})$ by $\partial(\mathbf{x})$.

Let $m \in \mathbb{N}_*^+$ and consider \mathbb{IR}^m . We call *box* an element of \mathbb{IR}^m and we will denote it by an uppercase bold letter as \mathbf{X} . Let $\mathbf{X} = (\mathbf{x}_1, \dots, \mathbf{x}_m)$ be an element of \mathbb{IR}^m , we will denote by $m(\mathbf{X})$ its center $(m(\mathbf{x}_1), \dots, m(\mathbf{x}_m))$ and by $w(\mathbf{X})$ its width defined as $w(\mathbf{X}) = max_{1 \leq i \leq m} w(\mathbf{x}_i)$. The interior $(]l(\mathbf{x}_1), u(\mathbf{x}_1)[, \dots,]l(\mathbf{x}_m), u(\mathbf{x}_m)[)$ of \mathbf{X} will be denoted by $int(\mathbf{X})$ and its boundary $\mathbf{X} \setminus int(\mathbf{X})$ by $\partial(\mathbf{X})$.

Usual arithmetic operators can be extended to interval and boxes.

2.2 Evaluating Functions on Boxes

Consider the polynomial function $f: \mathbb{R}^m \to \mathbb{R}$ and let $\mathbf{X} \in \mathbb{R}^m$. We will denote by $f(\mathbf{X})$ the set $\{f(X)|X \in \mathbf{X}\}$. The following definitions are picked up from [10].

We will call interval extension of f a function $\Box f : \mathbb{IR}^m \to \mathbb{IR}$ s.t.

$$\mathbf{X} \in \mathbb{IR}^m \Rightarrow f(\mathbf{X}) \subseteq \Box f(X)$$
 (1)

and

$$X \in \mathbb{R}^m \Rightarrow f(X) = \Box f(X). \tag{2}$$

We say that an interval extension $\Box f$ is inclusion monotonic if

$$\mathbf{X} \subseteq \mathbf{Y} \Rightarrow \Box f(\mathbf{X}) \subseteq \Box f(\mathbf{Y}). \tag{3}$$

For a polynomial f, a natural interval extension of f that is inclusion monotonic is obtained by combining interval operators that intervene in the Horner form of f (see [10]). We will denote it ${}^{0}f$, and ${}^{0}f(\mathbf{X})$ will be the value of the evaluation of ${}^{0}f$ on $\mathbf{X} \in \mathbb{IR}^{m}$.

An other inclusion monotonic interval extension (see [10]) that is classically used is the mean value form 1f defined as

$${}^{1}f(\mathbf{X}) = f(\mathbf{P}) + \Box J_{f}(\mathbf{X})(\mathbf{X} - \mathbf{P}) \tag{4}$$

where **P** is the center of **X** represented as an interval and $\Box J_f$ an inclusion monotonic interval extension of the Jacobian matrix J_f of f. 0J_f is classically used for $\Box J_f$.

Here we will use the interval extension obtained by considering Taylor expansion at order 2 around the center P of X, defined as:

$${}^{2}f(\mathbf{X}) = f(\mathbf{P}) + J_{f}(\mathbf{P})(\mathbf{X} - \mathbf{P}) + \frac{1}{2}(\mathbf{X} - \mathbf{P})^{t}({}^{0}H_{f}(\mathbf{X}))(\mathbf{X} - \mathbf{P})$$

$$\tag{5}$$

where ${}^{0}H_{f}$ is the natural interval extensions of the Hessian matrix H_{f} of f. ${}^{2}f$ is shown in [6] to be an inclusion monotonic interval extension of f, and we will call it evaluation at order two of f.

Above definitions are easily extended to functions $F: \mathbb{R}^m \to \mathbb{R}^m$. Notice that if $\Box F$ is an interval extension of F, then we have

$$0 \notin \Box F(\mathbf{X}) \Rightarrow F \text{ does not vanish on } \mathbf{X}.$$
 (6)

Algorithm 1 CertifyNoSolution(F, X)

Input: A function $F: \mathbb{R}^m \to \mathbb{R}^m$ and a box **X**.

Output: true or false; if true then F = 0 has no solution in X.

1: if $(0 \notin {}^{0}F(\mathbf{X}) \cap {}^{2}F(\mathbf{X}))$ or $({}^{2}K_{F}(\mathbf{X}) \cap \mathbf{X} = \emptyset)$ then

2: return true

3: return false

Algorithm 2 CertifyOneSolution(F, X)

Input: A function $F: \mathbb{R}^m \to \mathbb{R}^m$ and a box **X**.

Output: true or false; if true then X contains a unique solution of F = 0.

1: if ${}^2K_F(\mathbf{X}) \subset int(\mathbf{X})$ then

2: return true

3: return false

2.3 The Krawczyk Operator

We consider now a function $F: \mathbb{R}^m \to \mathbb{R}^m$ defined as $F(X) = (f_1(X), \dots, f_m(X))$ where $f_i: \mathbb{R}^m \to \mathbb{R}$ for $1 \le i \le m$ and we recall the definition of the Krawczyk operator K_F that is a classical tool in interval analysis (see for instance [2, Def. 1.16] or [4, Theo. 8.2] or [9, Sec. 7]).

$$K_F(\mathbf{X}) = \mathbf{P} - (J_F(\mathbf{P}))^{-1}F(\mathbf{P}) + (I - (J_F(\mathbf{P}))^{-1}\Box J_F(\mathbf{X}))(\mathbf{X} - \mathbf{P})$$
(7)

where **P** is the center of **X** represented as an interval and $\Box J_F$ is the interval extensions of the Jacobian matrix J_F of F. K_f has the following properties:

- (K_1) $K_F(\mathbf{X}) \subset int(\mathbf{X}) \Rightarrow F(X) = 0$ has one and only one solution in \mathbf{X} that is in $K_F(\mathbf{X})$
- (K_2) $K_F(\mathbf{X}) \cap \mathbf{X} = \emptyset \Rightarrow F(X) = 0$ has no solution in \mathbf{X}
- (K_3) if **X** and **Y** are s.t. $K_F(\mathbf{X}) \subset int(\mathbf{X})$ and $K_F(\mathbf{Y}) \subset int(\mathbf{Y})$ then $\mathbf{X} \cap \mathbf{Y} \neq \emptyset \Rightarrow \mathbf{X}$ and **Y** contain the same solution of F(X) = 0.

Proof of (K_3) : because K_F is *isotone* $(i.e. \mathbf{X} \subseteq \mathbf{Y} \Rightarrow K_F(\mathbf{X}) \subseteq K_F(\mathbf{Y}))$, see [3], one has $K_F(\mathbf{X} \cap \mathbf{Y}) \subset int(\mathbf{X} \cap \mathbf{Y})$ and $\mathbf{X} \cap \mathbf{Y}$ contains a unique solution. \square

When using a mean value extension of J_F around the center **P** of **X** to compute $\Box J_F(\mathbf{X})$ one can rewrite Eq. 7 as

$${}^{2}K_{F}(\mathbf{X}) = \mathbf{P} - (J_{F}(\mathbf{P}))^{-1}(F(\mathbf{P}) + \mathbf{H})$$
(8)

where **H** is a box in \mathbb{IR}^m which *i*-th component $\mathbf{h_i}$ is:

$$\mathbf{h_i} = (\mathbf{X} - \mathbf{P})^t (^0 H_{f_s}(\mathbf{X}))(\mathbf{X} - \mathbf{P}) \tag{9}$$

where ${}^{0}H_{f_{i}}$ is the natural interval extension of the Hessian matrix $H_{f_{i}}$ of f_{i} . We will call ${}^{2}K_{F}(\mathbf{X})$ the Krawczyk operator at order 2 since it uses second order partial derivatives of F; we assume here that it satisfies properties $(K_{1}), (K_{2})$ and (K_{3}) .

One can use (K_2) and Eq. 6 to justify Algo. 1 that certifies that a system F = 0 with $F : \mathbb{R}^m \to \mathbb{R}^m$ has no solutions on a box \mathbf{X} . (K_1) justifies Algo. 2 that certifies that F = 0 has a unique solution on \mathbf{X} . Algo. 3 decides if the solution of F = 0 contained in a box \mathbf{X} s.t. $K_F(\mathbf{X}) \subset int(\mathbf{X})$ is already contained in a box of a list \mathcal{L} containing boxes \mathbf{Y} s.t. $K_F(\mathbf{Y}) \subset int(\mathbf{Y})$. It is correct from (K_3) .

Algorithm 3 IsSolInList (F, X, \mathcal{L})

```
Input: A function F : \mathbb{R}^m \to \mathbb{R}^m, a box X and a list of boxes \mathcal{L} s.t. K_F(\mathbf{X}) \subset int(\mathbf{X}) and \forall \mathbf{Y} \in \mathcal{L}, K_F(\mathbf{Y}) \subset int(\mathbf{Y}).
```

Output: true or false; if true then the solution of F = 0 contained in X is in a box of \mathcal{L} .

- 1: for $Y \in \mathcal{L}$ do
- 2: if $X \cap Y \neq \emptyset$ then
- 3: return true
- 4: return false

3 Adapting Arithmetic Precision

Intervals are usually represented by their two bounds represented by floating points, and interval operators by operations on floating points with appropriated rounding policy. In what follows, we will call *precision* of the arithmetic the number of bits of the mantissa of floating points.

The branch and bound method we did implement uses recursive bisections of boxes until it is possible to certify either the absence or the existence and uniqueness of a solution in each box. Lack of accuracy can intervene during this process either when a box has a component that has roughly the smallest width allowed by the arithmetic precision (*i.e.* the bounds are consecutive floating points), or when accumulated rounding affects the inclusion isotonic nature of an interval extension. These cases have to be detected to avoid infinite computations. When they occur a common strategy is to double the arithmetic precision and to continue the computations.

We recall in 3.1 two criteria pickud up from [7] that decide if the arithmetic precision is not sufficient, and we present in 3.2 a criterion that is, as far as we know, new and is used as an heuristic in our solver.

3.1 Criteria of [7]

[7] presents a simple branch and bound algorithm using adaptive multi-precision to find zeros of an univariate real function f with interval extension $\Box f$, using interval newton method. At each step, an interval \mathbf{x} is bisected in $\mathbf{x}^1, \mathbf{x}^2$ s.t. $\mathbf{x} = \mathbf{x}^1 \cup \mathbf{x}^2$, and the arithmetic precision is increased if one of the following conditions holds:

- $w(\mathbf{x}^1) \ge w(\mathbf{x})$ or $w(\mathbf{x}^2) \ge w(\mathbf{x})$,
- $w(\Box f(\mathbf{x}^1)) \ge w(\Box f(\mathbf{x}))$ or $w(\Box f(\mathbf{x}^2)) \ge w(\Box f(\mathbf{x}))$.

Notice that the second criterion contradicts Eq. 1: $\Box f$ is not an interval extension of f due to numeric inaccuracy. We adapt here these criteria to a multi-variate context with $F: \mathbb{R}^m \to \mathbb{R}^m$, $\Box F: \mathbb{IR}^m \to \mathbb{IR}^m$ an interval extension of F, $\mathbf{X}_1, \mathbf{X}_2$ and \mathbf{X} elements of \mathbb{IR}^m such that $\mathbf{X} = \mathbf{X}_1 \cup \mathbf{X}_2$. In the branch and bound method presented in Sec. 4, the arithmetic precision is increased if one of the following conditions holds:

$$(C_1)$$
 $w(\mathbf{X}_1) \geq w(\mathbf{X})$ or $w(\mathbf{X}_2) \geq w(\mathbf{X})$,

$$(C_2)$$
 $w(\Box F(\mathbf{X}_1)) \ge w(\Box F(\mathbf{X}))$ or $w(\Box F(\mathbf{X}_2)) \ge w(\Box F(\mathbf{X}))$.

Algo. 4 verifies these conditions and returns **true** if (C_1) or (C_2) is satisfied.

Algorithm 4 CheckCond12(F or \mathcal{F} , X, X_1 , X_2)

Input: A function $F : \mathbb{R}^m \to \mathbb{R}^m$ or a list \mathcal{F} of functions $f : \mathbb{R}^m \to \mathbb{R}$, three boxes $\mathbf{X}, \mathbf{X_1}, \mathbf{X_2}$. Output: if (C_1) or (C_2) is satisfied then true; false otherwise.

Algorithm 5 CheckCond3(F,X)

Input: A function $F: \mathbb{R}^m \to \mathbb{R}^m$, a box **X**.

Output: if (C_3) is satisfied then true; false otherwise.

3.2 A new criterion

Consider Eqs. (7) and (8). Whatever its order (we state it here for order two), one can rewrite Krawczyk operator as

$${}^{2}K_{F}(\mathbf{X}) = -({}^{0}J_{F}(\mathbf{P}))^{-1}({}^{0}F(\mathbf{P})) + \mathbf{P} + \text{something}$$
(10)

to highlight that $F(\mathbf{P})$ and $J_F(\mathbf{P})$ are interval evaluations. Hence one has

$$w(^{2}K_{F}(\mathbf{X})) = w((^{0}J_{F}(\mathbf{P}))^{-1}(^{0}F(\mathbf{P}))) + w(\text{something})$$
(11)

and a necessary condition for ${}^2K_F(\mathbf{X})$ to certify the existence of a unique solution in \mathbf{X} is $w(({}^0J_F(\mathbf{P}))^{-1}({}^0F(\mathbf{P}))) < w(\mathbf{X})$: otherwise one can not have ${}^2K_F(\mathbf{X}) \subset int(\mathbf{X})$. Recall that \mathbf{P} is a point (i.e. $w(\mathbf{P}) = 0$) hence one should have, $w({}^0F(\mathbf{P})) = 0$ and $w(({}^0J_F(\mathbf{P}))^{-1}({}^0F(\mathbf{P}))) = 0$.

In the branch and bound method presented in Sec. 4, the arithmetic precision is increased if the following condition holds:

$$(C_3)$$
 $w((^0J_F(\mathbf{P}))^{-1}(^0F(\mathbf{P}))) \ge w(\mathbf{X})$ and $w(^0F(\mathbf{P})) \ge w(\mathbf{X})$.

In (C_3) , the condition $w({}^0F(\mathbf{P})) \geq w(\mathbf{X})$ is used to filter cases where $w(({}^0J_F(\mathbf{P}))^{-1}({}^0F(\mathbf{P}))) \geq w(\mathbf{X})$ is due to low values of partial derivatives of F in \mathbf{P} . In particular, when the latter condition holds, it contradicts Eq. 2 and 0F is not an interval extension of F due to numeric inaccuracy. Algo. 5 verifies this condition and returns **true** if it is satisfied.

This condition is used as an heuristic and is checked only if a maximal arithmetic precision specified by the user has not been reached.

4 Algorithm

We describe in Algo. 6 the adaptive multi-precision subdivision solver we implemented. Its input and output are fully specified in Sec. 4.1. For a given initial box \mathbf{X}_0 where solutions of F(X) = 0 are sought, a minimal width $\omega \in \mathbb{R}^+$ of boxes that can be explored, an initial arithmetic precision p and a maximal precision p_{max} , it proceeds as follows.

The simple branch and bound algorithm described in Algo. 7 is first applied to \mathbf{X}_0 using p as arithmetic precision. Its output are a list of boxes containing a unique solution of F(X) = 0, a list of boxes with width smaller than ω that can contain solutions and a list \mathcal{L}_{prec} of boxes such that one of the conditions (C_1) , (C_2) or (C_3) holds.

The precision p is then doubled and Algo. 7 is applied to boxes of \mathcal{L}_{prec} . This process is iterated until p reaches p_{max} . When Algo. 7 is applied for the last time with $p = p_{max}$, the condition (C_3) is not checked.

Sec. 4.2 describes Algo. 7.

Algorithm 6 Subdivision Solving With Adaptive Arithmetic Precision

Input: A function $F: \mathbb{R}^m \to \mathbb{R}^m$, a box \mathbf{X}_0 , a real number ω , an initial precision p, a maximal precision p_{max} as described in Sec 4.1.

```
Output: Two lists \mathcal{L}_{sols}, \mathcal{L}_{comp} and an integer r as described in Sec 4.1.
  1: Let \mathcal{L}_{sols}, \mathcal{L}'_{sols}, \mathcal{L}_{comp}, \mathcal{L}'_{comp} and \mathcal{L}_{prec} be empty lists.
  2: Push back (\mathbf{X}_0, \mathbf{true}) in \mathcal{L}_{prec}.
       while \mathcal{L}_{prec} is not empty and p \leq p_{max} do
               \begin{split} & (\mathcal{L}'_{sols}, \mathcal{L}'_{comp}, \mathcal{L}_{prec}) \leftarrow \texttt{SolveWithFixedPrec}(F, \mathcal{L}_{prec}, \omega, p, p_{max}) \\ & \texttt{Append boxes of } \mathcal{L}'_{sols} \texttt{ to } \mathcal{L}_{sols} \\ & \texttt{Append boxes of } \mathcal{L}'_{comp} \texttt{ to } \mathcal{L}_{comp} \end{split} 
  5:
  6:
               if 2p < p_{max} or p == p_{max} then
  7:
                      Set p to 2p
  8:
  9:
               else
                      Set p to p_{max}
10:
11: Determine r as described in Sec 4.1.
12: return \mathcal{L}_{sols}, \mathcal{L}_{comp}, r
```

4.1 Input and Output of Algo. 6

Our multi-precision branch and bound method accepts mainly as input:

- a polynomial function $F(X) = (f_1(X), \dots, f_m(X))$, where $X = (x_1, \dots, x_m)$;
- a box \mathbf{X}_0 where solutions of F(X) = 0 are sought;
- a real number $\omega \in \mathbb{R}^+$ that is the minimum width of boxes to be explored during the subdivision process;
- an initial precision p and a maximal precision p_{max} of the floating arithmetic used to represent bounds of intervals, given as the number of bits of the mantissa.

The minimal width ω allows to avoid infinite computations arising in particular when F(X) = 0 has non-regular solutions in \mathbf{X}_0 . If it is null, the termination of the process is not ensured.

The output of our multi-precision branch and bound method consists in:

- a list of boxes \mathcal{L}_{sols} containing solutions;
- a list of boxes \mathcal{L}_{comp} where other solutions could lie;
- an integer r specifying the status of the solving process.

Consider now the following properties:

- (P_1) if $\mathbf{X}_s \in \mathcal{L}_{sols}$ then it exists a unique $X_s \in \mathbf{X}_s \cap int(\mathbf{X}_0)$ s.t. $F(X_s) = 0$;
- (P_2) if $X_s \in int(\mathbf{X}_0)$ is s.t. $F(X_s) = 0$ then it exists at most one $\mathbf{X}_s \in \mathcal{L}_{sols}$ s.t. $X_s \in \mathbf{X}_s$;
- (P₃) if \mathcal{L}_{comp} is empty then for each $X_s \in int(\mathbf{X}_0)$ s.t. $F(X_s) = 0$ it exists $\mathbf{X}_s \in \mathcal{L}_{sols}$ s.t. $X_s \in \mathbf{X}_s$; furthermore there is no solution of F = 0 on $\partial(\mathbf{X}_0)$.

Properties (P_1) and (P_2) are always satisfied when the process terminates. When, in addition, (P_3) is satisfied, the value of r is 0. When (P_3) is not satisfied because of a lack of arithmetic precision, the value of r is 1. Otherwise the value of r is 2.

4.2 Branch and Bound Method with Fixed Arithmetic Precision

The branch and bound algorithm described in Algo. 7 can be seen as a Breadth First Search in a tree which root corresponds to an initial box X_0 , and children of a node corresponding to a box X correspond either to boxes obtained by bisecting X, *i.e.* cutting it in two boxes with respect to one of its components, or to a box obtained by contracting X around a solution.

The goal of such an algorithm is to find sub-boxes \mathbf{X} of \mathbf{X}_0 that contains a unique solution X_* of F=0 s.t. $X_* \in int(\mathbf{X}_0)$. Notice that the krawczyk test used in Algo. 2 can only certify existence and uniqueness of a solution in $int(\mathbf{X})$, and solutions lying exactly on borders of sub-boxes of \mathbf{X}_0 could be missed. ϵ -inflation introduced for instance in [10, Sec. 5.9] can among other circumvent this pitfall. It consists in slightly enlarging a box \mathbf{X} obtaining \mathbf{X}_{ϵ} s.t. $\mathbf{X} \subset \mathbf{X}_{\epsilon}$. Hence Algo. 2 is applied to \mathbf{X}_{ϵ} to certify existence and uniqueness of a solution in \mathbf{X}_{ϵ} . This mechanism can however lead to find the same solutions in several neighbor boxes. $X_* \in int(\mathbf{X}_0)$ is then verified when $\mathbf{X}_{\epsilon} \subseteq int(\mathbf{X}_0)$. In order to optimize the number of evaluations of F and its derivatives, the absence of solutions with Algo. 1 is also tested on \mathbf{X}_{ϵ} .

A leaf of the tree corresponds

- (n_1) either to a box **X** s.t. $w(\mathbf{X}) \leq \omega$ that can possibly contain solutions but that are smallest than the minimum width ω given in input,
- (n_2) or to a box X that is certified to contain no solution of F=0 with Algo. 1,
- (n_3) or to a box X s.t. X_{ϵ} contains a unique solution X_* of F=0 and $X_{\epsilon} \subseteq int(X_0)$.

An inner node of the tree corresponds

- (n_4) either to a box \mathbf{X} s.t. existence and uniqueness of a solution is certified in \mathbf{X}_{ϵ} , and s.t. $\mathbf{X}_{\epsilon} \cap \partial(\mathbf{X}_0) \neq \emptyset$; this case is identified in Algo. 7 with the boolean variable inflateAndBisect;
- (n_5) either to a box **X** where neither the absence nor the existence of a solution can be certified; such a node has two children corresponding to boxes obtained by bisecting **X**.

When a node corresponding to a box \mathbf{X} is visited, it is first checked with Algo. 8 that the actual arithmetic precision p is sufficient. If it is not, \mathbf{X} is pushed in the list \mathcal{L}_{prec} ; the subtree which root is the actual node will be explored with higher precision providing that $p < p_{max}$. Notice that the condition (C_3) presented in Sec. 3.2 is checked in Algo. 8 only if $p < p_{max}$.

If the arithmetic precision p is sufficient, the type of the actual node $((n_1)$ or (n_2) or ... or (n_5)) is determined. The actual node is of type (n_3) if $CertifyOneSolution(F, X_{\epsilon})$ returns true (see Algo. 2) and $X_{\epsilon} \subseteq int(X_0)$. If the latter condition is not fulfilled the actual node is of type (n_4) and the value of inflateAndBisect is set to false. The sole child of the actual node corresponds to the box ${}^2K_F(X_{\epsilon}) \subset X$. If $X_{\epsilon} \subseteq int(X_0)$, it is tested with Algo. 3 that the solution in X_{ϵ} has not already been found. Finally, when the actual node is of type (n_5) , X is bisected.

Literature proposes different strategies to choose a direction to cut a box \mathbf{X} , and some of them are surveyed in [1]. We did choose here to implement the maximum smear-diameter strategy (see [1, Sec. 3.1.1, $\mathbf{MaxSmearDiam}$]). In Algo. 7 the bisection is performed by the function $\mathbf{Bisect}(F, \mathbf{X}, \omega)$, where the direction i to cut $\mathbf{X} = (\mathbf{x}_1, \dots, \mathbf{x}_i, \dots, \mathbf{x}_m)$ is chosen so that $w(\mathbf{x}_i) > \omega$. The latter function returns a couple $(\mathbf{X}_1, \mathbf{X}_2)$ of boxes s.t. $\mathbf{X}_1 = (\mathbf{x}_1, \dots, [l(\mathbf{x}_i), m(\mathbf{x}_i)], \dots, \mathbf{x}_m)$ and $\mathbf{X}_2 = (\mathbf{x}_1, \dots, [m(\mathbf{x}_i), u(\mathbf{x}_i)], \dots, \mathbf{x}_m)$.

$\overline{\textbf{Algorithm 7}}$ SolveWithFixedPrec(F, \mathcal{L}_{work} , ω , p, p_{max})

```
Input: A function F: \mathbb{R}^m \to \mathbb{R}^m, a list \mathcal{L}_{work} of boxes, a real number \omega, a precision p and a
     maximal precision p_{max}.
Output: Three lists \mathcal{L}_{sols}, \mathcal{L}_{comp} and \mathcal{L}_{prec} of boxes.
 1: while \mathcal{L}_{work} is not empty do
           Pop the front of \mathcal{L}_{work} and store it in (\mathbf{X}, \mathtt{inflateAndBisect}).
           if {\tt CheckPrec}(F, \mathbf{X}, \omega, p, p_{max}, {\tt inflateAndBisect}) then
 3:
 4:
                 Push back X in \mathcal{L}_{prec}.
                continue
 5:
           if w(\mathbf{X}) \leq \omega then
 6:
                 Push back X in \mathcal{L}_{comp}.
 7:
                 continue
 8:
           if inflateAndBisect then
 9:
                 Let X_{\epsilon} be obtained by \epsilon-inflation of X.
10:
           else
11:
                 Let \mathbf{X}_{\epsilon} be a copy of \mathbf{X}.
12:
           if CertifyNoSolution(F, \mathbf{X}_{\epsilon}) then
13:
                 continue
14:
           if CertifyOneSolution(F, \mathbf{X}_{\epsilon}) then
15:
                 if \mathbf{X}_{\epsilon} \cap \partial(\mathbf{X}_0) \neq \emptyset then
16:
                      Push back ({}^{2}K_{F}(\mathbf{X}_{\epsilon}), false) in \mathcal{L}_{work}
17:
                 else if \mathbf{X}_{\epsilon} \subseteq int(\mathbf{X}_0) and not IsSolInList(F, \mathbf{X}_{\epsilon}, \mathcal{L}_{sols}) then
18:
                      Push back \mathbf{X}_{\epsilon} in \mathcal{L}_{sols}
19:
20:
           else
                 (\mathbf{X}_1,\mathbf{X}_2)=\mathtt{Bisect}(F,\mathbf{X},\omega).
21:
                 Push back (\mathbf{X}_1, \mathbf{true}) and (\mathbf{X}_2, \mathbf{true}) in \mathcal{L}_{work}.
22:
23: return \mathcal{L}_{sols}, \mathcal{L}_{comp}, \mathcal{L}_{prec}
```

5 Benchmarks

We propose here some experimental results to justify the chosen strategy for certifying non-existence or existence and uniqueness of a solution in a box. We compare four possible strategies for functions CertifyNoSolution and CertifyOneSolution:

- (1) Evaluation at order 2 and Krawczyk operator at order 2, as described in previous algorithms;
- (2) Evaluation at order 2 and Krawczyk operator as defined in Eq. 7: obtained by replacing ${}^{2}K_{F}(X)$ by $K_{F}(X)$ in previous algorithms;
- (3) Evaluation at order 1 and Krawczyk operator as defined in Eq. 7: obtained by replacing ${}^{2}F$ by ${}^{1}F$ and ${}^{2}K_{F}(X)$ by $K_{F}(X)$ in previous algorithms;
- (4) Natural interval extension and Krawczyk operator as defined in Eq. 7: obtained by replacing 2F by 0F and ${}^2K_F(X)$ by $K_F(X)$ in previous algorithms.

We did use these four strategies to solve dense, randomly generated, systems with m polynomial equations of degree d with integer coefficients of bit-size 8, for $(m, d) \in \{(2, 64), (2, 128), (3, 16), (3, 32), (4, 8), (5, 4)\}$. Table 1 gives for each strategy and each couple (m, d) the number n of boxes that have been explored and the sequential time t in seconds spent to solve the system.

Algorithm 8 CheckPrec(F, X, ω , p, p_{max} , inflateAndBisect)

Input: $F, \mathbf{X}, \omega, p, p_{max}$ as described in Sec. 4.1, and a boolean variable inflateAndBisect. Output: true if the arithmetic precision has to be increased to treat \mathbf{X} ; false otherwise.

- 1: if inflateAndBisect then
- 2: $(\mathbf{X}^1, \mathbf{X}^2) = \text{Bisect}(F, \mathbf{X}, \omega)$.
- 3: Let $\mathbf{X}_{\epsilon}, \mathbf{X}_{\epsilon}^{1}, \mathbf{X}_{\epsilon}^{2}$ be obtained by ϵ -inflation of $\mathbf{X}, \mathbf{X}^{1}, \mathbf{X}^{2}$.
- 4: return CheckCond12(F, X_{ϵ} , X_{ϵ}^{1} , X_{ϵ}^{2}) or (CheckCond3(F, X_{ϵ}) and $p < p_{max}$)
- 5: **else**
- 6: return (CheckCond3(F, \mathbf{X}) and $p < p_{max}$)

Table 1: Comparaison of strategies (1),(2),(3) and (4). m is the number of equations and variables of the system, d is the degree of its polynomial equations. n is the number of boxes that have been explored, t the sequential time in seconds spent for the process on a Intel(R) Core i7-5600U CPU @ $2.60 \mathrm{GHz}$.

m	2				3			4		5		
d	6	4	128		16		32		8		4	
	n	t	n	t	n	t	n	t	n	t	n	t
(1)	855	0.33	1028	1.75	6650	2.65	18310	61.5	49647	17.0	104373	10.7
(2)	886	0.40	1053	2.01	6943	3.16	18881	70.9	52501	20.3	110229	12.6
(3)	1158	0.36	1594	2.24	14338	4.05	47703	107	158076	36.4	298727	21.9
(4)	1286	0.40	1916	2.66	23219	6.62	102539	230	363274	81.3	576107	39.6

We note that using evaluation at order 2 (i.e. strategies (1) and (2) versus (3) and (4)) brought an important gain both in terms of number of boxes explored and time, and higher m and d are, higher is this gain. The gain allowed by Krawczyk operator at order 2 (strategy (1) versus strategy (2)) is more perceptible for small values of m and d. Notice that applying strategy (1) instead of strategy (2) does not induce additional evaluations since values of the Hessian matrix are computed for the evaluation at order 2.

References

- [1] Elke Just. Subdivision strategies for boxes in branch-and-bound nonlinear solvers and verification. *Mathematics in Computer Science*, 8(3-4):341–355, 2014.
- [2] R. Baker Kearfott. Rigorous global search: continuous problems. Nonconvex optimization and its applications. Kluwer Academic Publishers, Dordrecht, Boston, 1996.
- [3] R. Krawczyk. Interval iterations for including a set of solutions. *Computing*, 32(1):13–31, 1984.
- [4] Ramon E Moore, R Baker Kearfott, and Michael J Cloud. *Introduction to Interval Analysis*. Society for Industrial and Applied Mathematics, Philadelphia, PA, USA, 2009.
- [5] Guillaume Moroz. Fast polynomial evaluation and composition. Technical Report RT-0453, Inria Nancy Grand Est (Villers-lès-Nancy, France), July 2013.
- [6] Louis B Rall. Mean value and taylor forms in interval analysis. SIAM Journal on Mathematical Analysis, 14(2):223–238, 1983.

- [7] N. Revol. Interval newton iteration in multiple precision for the univariate case. Numerical Algorithms, 34(2-4):417-426, 2003.
- [8] Nathalie Revol and Fabrice Rouillier. Motivations for an arbitrary precision interval arithmetic and the mpfi library. *Reliable computing*, 11(4):275–290, 2005.
- [9] Siegfried M. Rump. Solving algebraic problems with high accuracy. In *Proc. of the symposium on A new approach to scientific computation*, pages 51–120, San Diego, CA, USA, 1983. Academic Press Professional, Inc.
- [10] Volker Stahl. Interval Methods for Bounding the Range of Polynomials and Solving Systems of Nonlinear Equations. PhD thesis, Johannes Kepler University, Linz, Austria, 1995.



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