

On sufficient conditions of the injectivity : development of a numerical test algorithm via interval analysis

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Abstract. This paper presents a new numerical algorithm based on interval analysis able to verify that a continuously differentiable function is injective. The efficiency of the method is demonstrated by illustrative examples. These examples have been treated by a C++ solver which is made available.

Keywords: Injectivity, Interval Analysis, Identifiability.

1. Introduction

The purpose of this paper is to present a new method based on guaranteed numerical computation able to verify that a function $f : \mathcal{A} \subset \mathbb{R}^n \rightarrow \mathbb{R}^p$ is injective, *i.e.* satisfies

$$\forall a_1 \in \mathcal{A}, \forall a_2 \in \mathcal{A}, a_1 \neq a_2 \Rightarrow f(a_1) \neq f(a_2). \quad (1)$$

To our knowledge, it does not exist any numerical method able to perform this injectivity test. Moreover, the complexity of the algebraic manipulations involved often makes formal calculus in fault.

Note that the basic idea coming to mind which consists in verifying that the Jacobian matrix of f is injective is not a sufficient condition for injectivity as illustrated by the following example. Consider the function f defined by

$$f : \begin{cases} [-\pi, 2\pi] & \rightarrow \mathbb{R}^2 \\ x & \rightarrow \begin{pmatrix} \cos x \\ \sin x \end{pmatrix} \end{cases} \quad (2)$$

depicted on Figure (1). Its Jacobian matrix $Df(x)$ is

$$Df(x) = \begin{pmatrix} -\sin x \\ \cos x \end{pmatrix} \left(\neq \begin{pmatrix} 0 \\ 0 \end{pmatrix} \right).$$

Although, $Df(x)$ is full rank column ($\forall x \in [-\pi, 2\pi]$), the function f is not injective.

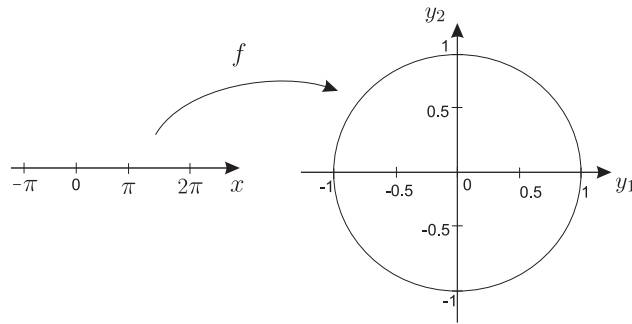


Figure 1. Graph of function f .

Many problems could be formulated as the injectivity verification of a specific function. For example, concerning the identification of parametric models, the problem of proving structural identifiability of parametric system amounts to checking the injectivity of the model structure (E.Walter and Pronzato, 1990; Ollivier, 1990). Other examples can be cited as in blind source separation, where the separability and the blind identifiability (Lagrange, 2005) consist in verifying the injectivity of particular functions.

In the context on structural identifiability, Braems and his collaborators presented in (Braems et al., 2001) an ε -approximation method that verifies the injectivity, namely ε -injectivity. It consists in verifying the following condition

$$\forall a_1 \in \mathcal{A}, \forall a_2 \in \mathcal{A}, |a_1 - a_2| > \varepsilon \Rightarrow f(a_1) - f(a_2) \neq 0, \quad (3)$$

which can be view as an approximation of the condition (1).

In this paper, we present a new algorithm, based on interval analysis, able to check that a function is injective. The paper is organized as follows. Section 2 presents interval analysis that will be used to check the injectivity. In Section 3, a new definition of partial injectivity in a domain makes possible to use interval analysis techniques to get a guaranteed answer. Section 4 presents an algorithm able to test a given function for injectivity. Finally, in order to show the efficiency of the algorithm, two illustrative examples are provided. A solver called ITVIA (Injectivity Test Via Interval Analysis) implemented in C++ is made available at <http://www.istia.univ-angers.fr/~lagrange/>.

2. Interval analysis

This section introduces some notions of interval analysis to be used in this paper.

A vector interval or a box $[x]$ of \mathbb{R}^n is defined by

$$[x] = [\underline{x}, \bar{x}] = \{x \in \mathbb{R}^n \mid \underline{x} \leq x \leq \bar{x}\}, \quad (4)$$

where the partial order \leq is understood componentwise and \underline{x} and \bar{x} are two elements of \mathbb{R}^n such that $\underline{x} \leq \bar{x}$. The set of all bounded boxes of \mathbb{R}^n will be denoted by $\mathbb{I}\mathbb{R}^n$. The enveloping box or hull box $[A]$ of a bounded subset $A \in \mathbb{R}^n$ is the smallest box of $\mathbb{I}\mathbb{R}^n$ that contains A . Figure 2 presents the hull box of a subset of \mathbb{R}^2 .

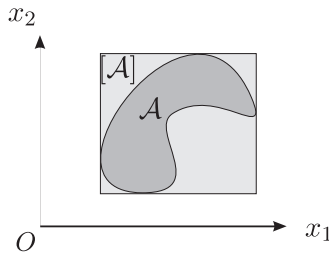


Figure 2. A hull box $[A]$ of a subset $A \in \mathbb{R}^2$.

By extension, an interval matrix $[M] = [\underline{M}, \overline{M}]$ is a set of matrices of the form :

$$[M] = \{M \in \mathbb{R}^{n \times m} \mid \underline{M} \leq M \leq \overline{M}\} \quad (5)$$

and $\mathbb{I}\mathbb{R}^{n \times m}$ denoted the set of all interval matrices of $\mathbb{R}^{n \times m}$. The properties of punctual matrices can naturally be extended to interval matrices. For example, $[M]$ is full column rank if all the matrices $M \in [M]$ are full column rank.

Interval arithmetic defined in (Moore, 1966) provides an effective method to extend all concepts of vector arithmetic to boxes.

Let $f : \mathbb{R}^n \rightarrow \mathbb{R}^m$ be a vector function; the set-valued function $[f] : \mathbb{I}\mathbb{R}^n \rightarrow \mathbb{I}\mathbb{R}^m$ is a *inclusion function* of f if, for any box $[x]$ of $\mathbb{I}\mathbb{R}^n$, it satisfies $f([x]) \subset [f]([x])$ (see Figure 3). Note that $f([x])$ is usually not a box contrary to $[f]([x])$. Moreover, since $[f([x])]$ is the hull box of $f([x])$, one has

$$f([x]) \subset [f([x])] \subset [f]([x]). \quad (6)$$

REMARK 1. *The computation of an inclusion function $[f]$ for any analytical function f can be obtained by replacing each elementary operator and function by its interval counterpart (Moore, 1966; Neumaier, 1990).*

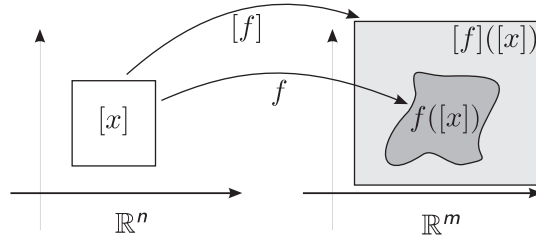


Figure 3. Inclusion function $[f]$ of a function f .

EXAMPLE 2. An inclusion function for

$$f : \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \rightarrow \begin{pmatrix} x_1^2 + x_2^2 \\ \cos(x_1 x_2) \end{pmatrix} \quad (7)$$

is

$$[f] : \begin{pmatrix} [x_1] \\ [x_2] \end{pmatrix} \rightarrow \begin{pmatrix} [x_1]^2 + [x_2]^2 \\ \cos([x_1] \times [x_2]) \end{pmatrix}. \quad (8)$$

If, for instance, $[x] = ([-1, 1], [0, \frac{\pi}{2}])^T$ then the box $[f]([x])$ is computed as follows:

$$[f]([x]) = \begin{pmatrix} [-1, 1]^2 + [0, \frac{\pi}{2}]^2 \\ \cos([-1, 1] \times [0, \frac{\pi}{2}]) \end{pmatrix} \quad (9)$$

$$= \begin{pmatrix} [0, 1] + [0, \frac{\pi^2}{4}] \\ \cos([- \frac{\pi}{2}, \frac{\pi}{2}]) \end{pmatrix} \quad (10)$$

$$= \begin{pmatrix} [0, 1 + \frac{\pi^2}{4}] \\ [0, 1] \end{pmatrix}. \quad (11)$$

Note that the operators $+$, \times , and functions \cos and $(.)^2$ in (8) are interval counterparts of those in (7).

3. Injectivity

This section presents some useful results concerning injective functions. Some definitions and fundamental results, based of the injectivity test, are introduced.

3.1. DEFINITION

Let us introduce the definition of *partial injectivity* of a function.

DEFINITION 1. Consider a function $f : \mathcal{A} \rightarrow \mathcal{B}$ and any set $\mathcal{A}_1 \subseteq \mathcal{A}$. The function f is said to be a *partial injection of \mathcal{A}_1 over \mathcal{A}* , noted $(\mathcal{A}_1, \mathcal{A})$ -injective, if $\forall a_1 \in \mathcal{A}_1, \forall a \in \mathcal{A}$,

$$a_1 \neq a \Rightarrow f(a_1) \neq f(a). \quad (12)$$

f is said to be \mathcal{A} -injective if it is $(\mathcal{A}, \mathcal{A})$ -injective.

EXAMPLE 3. Consider the three functions of Figure 4. The functions f_1 and f_2 are $([x_1], [x])$ -injective (although f_2 is not $[x]$ -injective) whereas f_3 is not.

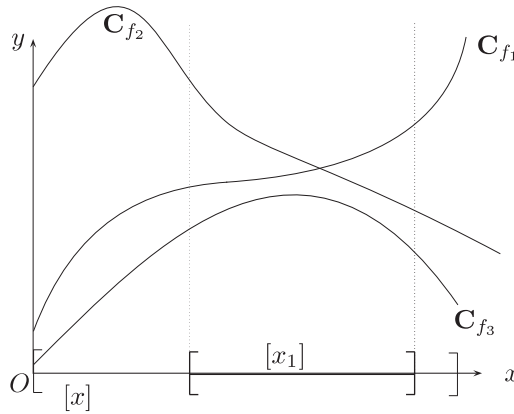


Figure 4. Graphs of functions f_1, f_2 and f_3 .

The following theorem motivates the implementation of the algorithm presented in Section 4.

THEOREM 4. Consider a function $f : \mathcal{A} \rightarrow \mathcal{B}$ and $\mathcal{A}_1, \dots, \mathcal{A}_p$ a collection of subsets of \mathcal{A} . We have

$$\forall i, 1 \leq i \leq p, f \text{ is } (\mathcal{A}_i, \mathcal{A}) \text{ - injective} \Leftrightarrow f \text{ is } \left(\bigcup_{i=1}^p \mathcal{A}_i, \mathcal{A} \right) \text{ - injective.} \quad (13)$$

Proof. (\Rightarrow) One has $\forall a_i \in \mathcal{A}_i, \forall a \in \mathcal{A}, a_i \neq a \Rightarrow f(a_i) \neq f(a)$. Hence $\forall b \in (\cup_i \mathcal{A}_i), \forall a \in \mathcal{A}, b \neq a \Rightarrow f(b) \neq f(a)$.

(\Leftarrow) Direct consequence of Definition 1. ■

3.2. PARTIAL INJECTIVITY CONDITION

In this paragraph, a fundamental theorem which gives a sufficient condition of partial injectivity, is proposed. First, let us introduce a generalization of the mean value theorem.

THEOREM 5 (Generalized Mean Value Theorem). *Consider a continuously differentiable function $f : \mathcal{A} \subseteq \mathbb{R}^n \rightarrow \mathbb{R}^m$. Let Df be its Jacobian matrix and $[x] \subset \mathcal{A}$. One has*

$$\forall a, b \in [x], \exists J_f \in [Df([x])] \text{ such that } f(b) - f(a) = J_f \cdot (b - a), \quad (14)$$

where $[Df([x])]$ denotes the hull box of $Df([x])$.

Proof. According to Mean-Value Theorem¹ (Kaplan, 1991) applied on each components $f_i : \mathbb{R}^n \rightarrow \mathbb{R}$ of f ($1 \leq i \leq m$) and since the segment $seg(a, b)$ belongs to $[x]$, we have

$$\exists \xi_i \in [x] \text{ such that } f_i(b) - f_i(a) = Df_i(\xi_i) \cdot (b - a). \quad (15)$$

Taking $J_{f_i} = Df_i(\xi_i)$, we get

$$\exists J_{f_i} \in Df_i([x]) \text{ such that } f_i(b) - f_i(a) = J_{f_i} \cdot (b - a). \quad (16)$$

Thus

$$\exists J_f \in \begin{pmatrix} Df_1([x]) \\ \vdots \\ Df_m([x]) \end{pmatrix} \text{ such that } f(b) - f(a) = J_f \cdot (b - a). \quad (17)$$

i.e., since $(Df_1([x]), \dots, Df_m([x]))^T \subset [Df([x])]$ (see Equation (6)),

$$\exists J_f \in [Df([x])] \text{ such that } f(b) - f(a) = J_f \cdot (b - a). \quad (18)$$

■

EXAMPLE 6. *Consider the function*

$$f : \begin{cases} \mathbb{R} & \rightarrow & \mathbb{R}^2 \\ x & \rightarrow & (y_1, y_2)^T \end{cases} . \quad (19)$$

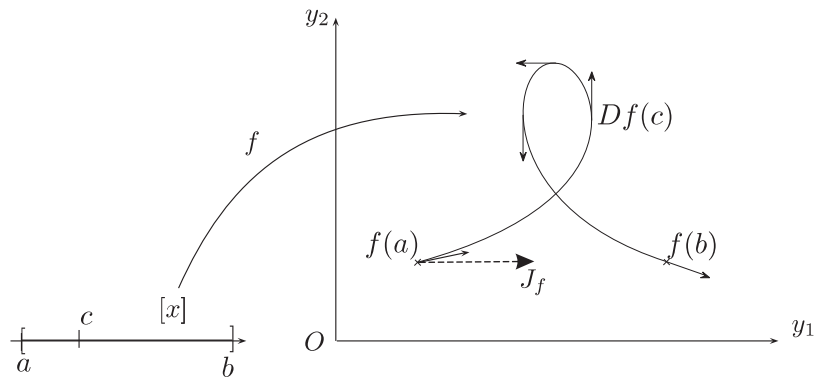


Figure 5. Graph of $f : \mathbb{R} \rightarrow \mathbb{R}^2$.

depicted in Figure 5. Figure 6 represents the set $Df([x])$ of all derivatives of f (drawn as vectors) and its hull box $[Df([x])]$. One can see that the vector J_f defined in (14) belongs to $[Df([x])]$ (but $J_f \notin Df([x])$) as forecasted by Theorem 5.

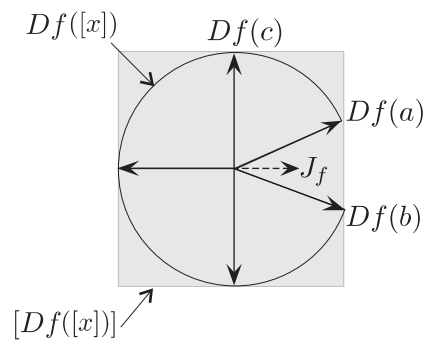


Figure 6. Illustration of the set $[Df([x])]$.

Now, the following theorem introduces a sufficient condition of partial injectivity. This condition will be exploited in next section in order to design a suitable algorithm that test injectivity.

¹ Let $f : U \subset \mathbb{R}^n \rightarrow \mathbb{R}$ be a differentiable function. If a and b belong to U such that the segment between a and b , noted $seg(a, b)$, is included in U . Then, there exists ξ belonging to $seg(a, b)$ such that

$$f(b) - f(a) = Df(\xi) \cdot (b - a).$$

THEOREM 7. *Let $f : \mathcal{A} \subset \mathbb{R}^n \rightarrow \mathbb{R}^m$ be a continuously differentiable function and $[x_1] \subset [x] \subset \mathcal{A}$. Set $[\tilde{x}] = [f^{-1}(f([x_1])) \cap [x]]$. If the interval matrix $[Df([\tilde{x})]$ is full column rank then f is $([x_1], [x])$ -injective.*

Proof. The proof is by contradiction.

Assume that f is not $([x_1], [x])$ -injective then

$$\exists b \in [x_1], \exists a \in [x] \text{ such that } b \neq a \text{ and } f(b) = f(a). \quad (20)$$

Now, since $f(a) = f(b)$, one has $a \in f^{-1}(f([x_1])) \cap [x]$ and trivially $b \in f^{-1}(f([x_1])) \cap [x]$. Therefore, since $f^{-1}(f([x_1])) \cap [x] \subset [f^{-1}(f([x_1])) \cap [x]] = [\tilde{x}]$ (see Equation (6)), one has $a, b \in [\tilde{x}]$.

Hence, (20) implies

$$\exists a, \exists b \in [\tilde{x}], \text{ such that } b \neq a \text{ and } f(b) = f(a). \quad (21)$$

To conclude, according to Theorem 5, $\exists a, \exists b \in [\tilde{x}]$,

$\exists J_f \in [Df([\tilde{x})]$ such that

$$b \neq a \text{ and } 0 = f(b) - f(a) = J_f \cdot (b - a), \quad (22)$$

i.e. $\exists J_f \in [Df([\tilde{x})]$ such that J_f is not full column rank and therefore the (interval) matrix $[Df([\tilde{x})]$ is not full column rank. ■

4. ITVIA Algorithm

In this section, we present the Injectivity Test's Via Interval Analysis algorithm designed from Theorems 4 and 7. This algorithm test the injectivity of a given continuously differentiable function $f : \mathbb{R}^n \rightarrow \mathbb{R}^m$ ($f \in \mathcal{C}^1$) over a given box $[x]$.

ITVIA can be decomposed into two distinct algorithms :

- Algorithm 1 checks if the interval matrix $[Df([f^{-1}(f([x_1])) \cap [x])]$ is full column rank. In the positive case, according to Theorem 7, the function f is $([x_1], [x])$ -injective. Therefore, Algorithm 1 can be viewed as a test for partial injectivity.
- Algorithm 2 divides the initial box $[x]$ into a paving² $\{[x_i]\}_i$ such that, for all i , the function f is $([x_i], [x])$ -injective. Then, since $[x] = (\cup_i [x_i])$ and according to Theorem 4, f is $[x]$ -injective.

In Algorithm 1 a set inversion technique (Goldsztein, 2005; Jaulin et al., 2001) is first exploited to characterize a box $[\tilde{x}]$ that contain

² A paving of $[x]$ is a finite set of non-overlapping boxes $\{[x_i]\}_i$ such that $[x] = \bigcup_i [x_i]$

Algorithm 1 Partial_Injection

Require: f a C^1 function, $[x]$ the initial box and $[x_1]$ a box included in $[x]$.

Ensure: A boolean :

- *true* : f is $([x_1], [x])$ -injective,
- *false* : f may or not be partially injective.

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1: Initialization :  $\mathcal{L}_{stack} := \{[x]\}$ ,  $[\tilde{x}] := \emptyset$ .
2: while  $\mathcal{L}_{stack} \neq \emptyset$  do
3:   Pop  $\mathcal{L}_{stack}$  into  $[w]$ .
4:   if  $[f]([w]) \cap [f]([x_1]) \neq \emptyset$  then
5:     if  $\text{width}([w]) > \text{width}([x_1])$  then
6:       Bisect  $[w]$  into  $[w_1]$  and  $[w_2]$ .
7:       Stack  $[w_1]$  and  $[w_2]$  in  $\mathcal{L}_{stack}$ .
8:     else
9:        $[\tilde{x}] = [[\tilde{x}] \cup [w]]$ .
10:    end if
11:  end if
12: end while
13: if  $[Df]([\tilde{x}])$  is full column rank then
14:   Return true \ \ "  $f$  is  $([x_1], [x])$ -injective"
15: else
16:   Return False \ \ "Failure"
17: end if

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$[f^{-1}(f([x_1])) \cap [x]]$. The purpose of the condition in Step 5 is to avoid useless splitting of $[w]$ *ad infinitum*. Secondly, an interval arithmetic evaluation of Df over $[\tilde{x}]$ is performed in order to test the full ranking of the resulting matrix $[Df]([\tilde{x}])$. Thus, since $[Df]([\tilde{x}]) \subset [Df]([x])$ (see Equation (6)) and according to Theorem 7, if $[Df]([\tilde{x}])$ is full column rank, then f is $([x_1], [x])$ -injective.

There exists different sufficient conditions able to verify that a given matrix $[A]$ is full rank (Step 13). As usual, using interval analysis, one can basically use standard methods. For example, if $[A]$ is a square matrix, one can compute the (interval) determinant of $[A]$ or use the Interval Gauss Algorithm (Neumaier, 1990). In practice, those methods are seldom able to decide either or not a given matrix is full rank due to well known effect of multioccurrences.

To check a matrix is full rank, one can use the following theorem :

THEOREM 8. *Let $[A]$ be a $n \times m$ interval matrix and A be a $n \times m$ matrix with $n \leq m$. If $[\tilde{I}] = [A](A^T A)^{-1}A^T$ is strictly diagonally dominant then $[A]$ is full rank.*

Proof. The matrix $[\tilde{I}]$ is of dimension $n \times n$ and strictly diagonally dominant. Therefore, $[\tilde{I}]$ is invertible and of rank n . In general, one has for all matrices B_1 and B_2 , $\text{rank}(B_1 B_2) \leq \min(\text{rank}(B_1), \text{rank}(B_2))$. Hence,

$$n = \text{rank}([\tilde{I}]) \leq \min(\text{rank}([A]), \text{rank}((A^T A)^{-1}A^T)) \leq \text{rank}([A]) \leq n.$$

Then $[A]$ is full rank. ■

REMARK 9. *Note that $(A^T A)^{-1}A^T$ is the pseudoinverse of A . In practice (to apply Theorem 8) A is chosen to be the center of $[A]$. As a consequence, $[\tilde{I}]$ is often close to I that is to say, $[\tilde{I}]$ is diagonal dominant.*

Algorithm 2 Injectivity Test Via Interval Analysis

Require: f a \mathcal{C}^1 function and $[x]$ the initial box.

- 1: Initialization : $\mathcal{L} := \{[x]\}$.
 - 2: **while** $\mathcal{L} \neq \emptyset$ **do**
 - 3: Pull $[w]$ in \mathcal{L} .
 - 4: **if** $\text{Partial_Injection}(f, [x], [w]) = \text{False}$ **then**
 - 5: Bisect $[w]$ into $[w_1]$ and $[w_2]$.
 - 6: Push $[w_1]$ and $[w_2]$ in \mathcal{L} .
 - 7: **end if**
 - 8: **end while**
 - 9: Return " f is injective over $[x]$ ".
-

Algorithm 2 creates a paving of the initial box $[x]$ such that, for all i , the function f is $([x_i], [x])$ -injective. Therefore, if the algorithm terminates, then f is proved to be injective over $[x]$. Otherwise, the algorithm can be stopped (manually or with a ε condition on the width of boxes $[x_i]$ which remain to be tested). In this case, two domains are obtained : *An undetermined domain* composed of all the boxes in \mathcal{L} not proved partially injective and *a partial injective domain* anywhere else in $[x]$.

By combination of those algorithms, we can prove that a function is injective over a box $[x]$. A solver, called ITVIA, developed in C++ is made available and tests the injectivity of a given function $f : \mathbb{R}^2 \rightarrow \mathbb{R}^2$ (or $f : \mathbb{R} \rightarrow \mathbb{R}^2$) over a given box $[x]$.

5. Examples

In this section, two examples are provided in order to illustrate the efficiency of the solver ITVIA presented in previous section. We check the injectivity of two functions $f : \mathbb{R}^2 \rightarrow \mathbb{R}^2$ over a given box $[x]$.

5.1. M FUNCTION

Consider the function f , depicted in Figure 7, defined by

$$f : \begin{cases} \mathbb{R}^2 & \rightarrow \mathbb{R}^2 \\ \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} & \rightarrow \begin{pmatrix} y_1 \\ y_2 \end{pmatrix} = \begin{pmatrix} x_1 - x_2(x_1 \cos(x_1) + \sin(x_1)) \\ x_1 \sin(x_1) + x_2 \end{pmatrix} \end{cases} \quad (23)$$

and test its injectivity over the box $[x] = \left([-4, 4], [0, \frac{2}{10}]\right)^T$.

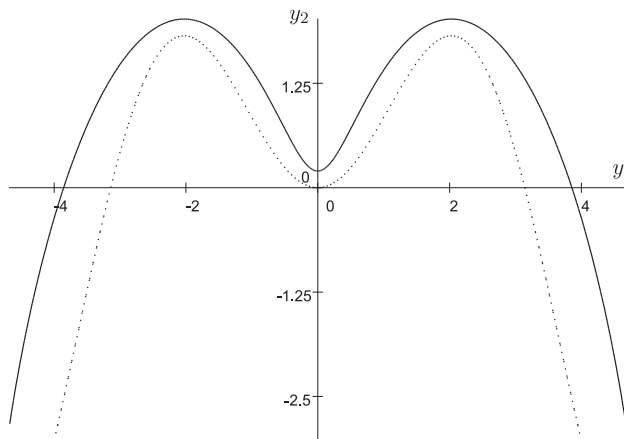


Figure 7. The image of the function f defined in (23) is depicted in dash for $x_1 \in [-4, 4]$ and $x_2 = 0$ and in black for $x_1 \in [-4, 4]$ and $x_2 = \frac{2}{10}$.

After less than 0.1 sec on a Pentium 1.7GHz, ITVIA proved that f is injective over $[x]$. The initial box $[x]$ has been cut out in a set of sub-boxes where f is partially injective. Figure 8 shows the successive bisections of $[x]$ made by ITVIA.

5.2. RIBBON FUNCTION

Consider the ribbon function f (depicted in Figure 9) defined by

$$f : \begin{cases} \mathbb{R}^2 & \rightarrow \mathbb{R}^2 \\ \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} & \rightarrow \begin{pmatrix} y_1 \\ y_2 \end{pmatrix} = \begin{pmatrix} \frac{x_1}{2} + (1 - x_2) \cos(x_1) \\ (1 - x_2) \sin(x_1) \end{pmatrix} \end{cases} \quad (24)$$

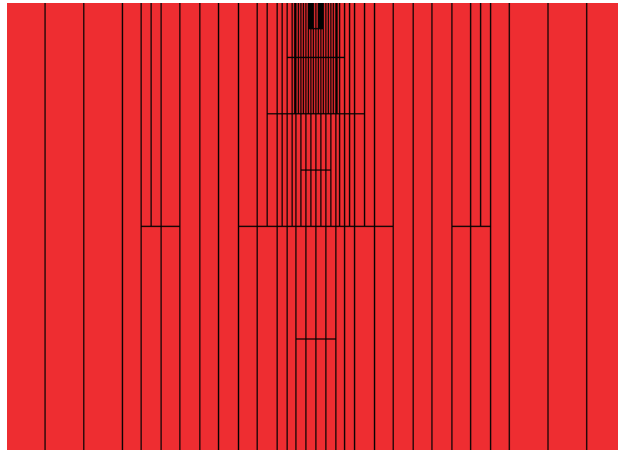


Figure 8. Bisection of $[x]$ obtained by ITVIA for the function f defined in (23). In gray, the partial injectivity domain and, in white, the indeterminate domain (empty in this example).

and get interest with its injectivity over the box $[x] = ([-1, 4], [0, \frac{1}{10}])^T$. Since the ribbon overlaps (see Figure 9), one can see that f is not injective over $[x]$.

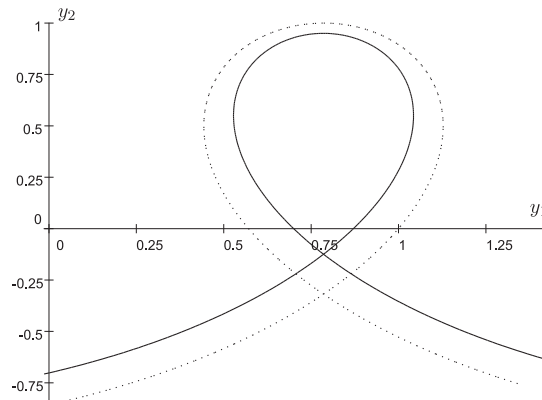


Figure 9. The function f defined in (24) is depicted in dash for $x_1 \in [-1, 4]$ and $x_2 = 0$ and in black for $x_1 \in [-1, 4]$ and $x_2 = \frac{1}{10}$.

After 3 seconds, the solver ITVIA is stopped (before going to end). It returns the solution presented in Figure 10. The function f has been proved to be a partial injection on the gray domain over $[x]$, whereas the white domain corresponds to the undeterminate domain where ITVIA was not able to prove the partial injectivity. Indeed, the indeterminate

domain corresponds to the non injective zone of f where all points are mapped in the overlapping zone of the ribbon.



Figure 10. Partition of the box $[x]$ obtained by ITVIA for the function f defined in (24). In gray, the partial injectivity domain and in white the indeterminate domain.

6. Conclusion

In this paper, we have presented a new algorithm able to test functions for injectivity generalizing the work presented in (Braems et al., 2001) restricted to ε -injectivity. Since interval analysis technics are used, the injectivity test is guaranteed.

In case of functions $f : \mathbb{R} \rightarrow \mathbb{R}^2$ and $f : \mathbb{R}^2 \rightarrow \mathbb{R}^2$, the solver ITVIA developed in C++ is available. From a given function f and a given box $[x]$, the solver partitiones $[x]$ into two domains : Partially injective domain and indeterminate domain (where the function may or not be injective). Of course, when the indetermined domain is empty, the function is injective over $[x]$.

In order to fill out this work, different perspectives appear. First of all, it will be interesting to improve the efficiency of the algorithm ITVIA by the additional use of constraint propagation. Secondly, we showed that the initial domain can be divided into two subsets where the function has only one preimage (*i.e.* where f is a partial injection) and where the function have more than one preimages. It will be attractive to pursue this work in order to divided initial domain in subsets where the function has a fixed number of preimages.

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