

Rigorous Inner Approximation of the Range of Functions

Alexandre Goldsztejn*
University of California, Irvine
Irvine CA, USA
agoldy@ics.uci.edu

Wayne Hayes
University of California, Irvine
Irvine CA, USA
wayne@ics.uci.edu

Abstract

A basic problem of interval analysis is the computation of a superset of the image of an interval by a function, called an outer enclosure. Here we consider the computation of an inner enclosure, which is a subset of the image. Inner approximations are harder than the outer ones in general: proving that a box is inside the image is actually equivalent to proving existence of solutions for a collection of systems of equations. Based on this remark, a new construction of the inner approximation is proposed. Then, it is shown that one can apply these ideas in the context of ordinary differential equations, hence providing some tools of potential interest for the theory of shadowing in dynamical systems.

1 Introduction

Interval analysis is naturally used to construct subsets (also called *outer approximations, enclosures*) of the range of real functions, i.e. intervals that rigorously contain the image of some domain by the function (see [12, 8] for some introduction to interval analysis). Constructing inner approximations of the range of a real function—i.e., intervals that are rigorously contained inside the image of some domain by the function—needs additional developments. Although many authors have investigated the construction of inner approximations in the case of functions $f : \mathbb{R}^n \rightarrow \mathbb{R}$ (see [25, 22] and references therein), a lot of work remains in the case of vector-valued functions $f : \mathbb{R}^n \rightarrow \mathbb{R}^m$. There is a direct relationship between inner approximation and existence theorems for systems of equations. Indeed, if one is able to build an inner approximation $\mathcal{I} \subseteq \text{range}(f, \mathbf{x})$ then $0 \in \mathcal{I}$ is obviously a sufficient condition for $\exists x \in \mathbf{x} f(x) = 0$. On the other hand, it seems that many existence theorems can naturally be used in order to build some inner approximation: defining $g_z(x) = f(x) - z$, $\mathcal{I} \subseteq \text{range}(f, \mathbf{x})$ holds if $g_z(x)$ is

*This work was done mainly while the first author was a post-doctoral fellow at the University of Central Arkansas.

proved to have a zero in \mathbf{x} for all $z \in \mathcal{I}$. Hence, a parameterized version of an existence theorem would be useful.

This observation leads to a branch and prune algorithm [6], hence allowing inner approximation of the range of vector valued functions $f : \mathbb{R}^n \rightarrow \mathbb{R}^n$. Such bisection algorithms are not well suited when the dimension of the image is not small, or when the evaluation of the function and its derivatives are expensive. In these cases, it may be useful to build an inner approximation of a small interval domain in one computation, in a similar way as the mean-value extension to intervals provides an outer approximation in one computation. The present paper provides such a construction. Thus, when the interval domain is small enough (roughly speaking when the mean-value extension computes an accurate outer approximation) one will be able to build both inner and outer approximations of the image of the interval domain by a function $f : \mathbb{R}^n \rightarrow \mathbb{R}^n$. To this end, we need only an interval enclosure of the image of the center of the domain, and an interval Lipschitz matrix for the whole domain. Hence, the inner approximation comes for almost no additional computational cost beyond that of the outer approximation.

Some potential applications of such inner approximations are foreseen in the context of shadowing dynamical systems [9]. Therefore, some techniques dedicated to the computation of some Lipschitz interval matrix of the solution to the IVP with respect to the initial condition are presented in a last section. In this context, the computation of a Lipschitz interval matrix involves the evaluation of the Taylor expansion (of dimension $n^2 + n$), and is hence very expensive. Computing an inner approximation for the same cost as the outer approximation is therefore very valuable in this context.

2 Interval Analysis

We assume a familiarity with basic interval analysis [11, 8, 17, 1, 20, 10]. Following [13], intervals, interval vectors and matrices are denoted by boldface letters.

Definition 1 (Lipschitz interval matrix (LIM)). Let $\phi :$

$\mathbb{R}^n \longrightarrow \mathbb{R}^m$ be a continuous function and $\mathbb{Y} \subseteq \mathbb{R}^n$. The interval matrix $\mathbf{J} \in \mathbb{IR}^{n \times m}$ is a LIM for ϕ and \mathbb{Y} if and only if

$$(\forall x, y \in \mathbb{Y})(\phi(x) - \phi(y) \in \mathbf{J} \cdot (x - y)), \quad (1)$$

or equivalently

$$(\forall x, y \in \mathbb{Y})(\exists J \in \mathbf{J})(\phi(x) - \phi(y) = J \cdot (x - y)). \quad (2)$$

The existence of a LIM \mathbf{J} for ϕ and \mathbb{Y} implies that the function is Lipschitz inside \mathbb{Y} with constant $\|\mathbf{J}\|$. If ϕ is continuously differentiable then

$$\left. \frac{\partial \phi(x)}{\partial x} \right|_y, \quad (3)$$

i.e. the partial derivative of $\phi(x)$ with respect to x evaluated at y , is denoted by $\phi'(y)$ when no confusion is possible. In this case, it is well known that any interval matrix that contains $\{\phi'(x) \mid x \in \mathbb{Y}\}$ is a LIM for ϕ and \mathbb{Y} [20]. Let us also recall that a LIM gives rise to the following interval enclosure (usually called the *mean-value extention*):

$$\text{Range}(f, \mathbf{x}) \subseteq f(\tilde{x}) + \mathbf{J} \cdot (\mathbf{x} - \tilde{x}), \quad (4)$$

where \mathbf{J} is a LIM for f and $\mathbf{x} \in \mathbb{IR}^n$ and $\tilde{x} \in \mathbf{x}$.

3 Inner and Outer Approximations of the Range of Real Functions

This section presents an inner approximation process for functions $f : \mathbb{R}^n \longrightarrow \mathbb{R}^n$. First box (i.e. axis-aligned interval vector) approximations are constructed. Then, more general parallelepipeds are used to allow inner approximation in a wider set of situations.

3.1 Box approximations

The well-known Poincaré-Miranda theorem (cf. [23]¹) is a generalization of the Intermediate Value Theorem to continuous function $f : \mathbb{R}^n \longrightarrow \mathbb{R}^n$. Interval analysis is very well suited to a rigorous application of the Poincaré-Miranda theorem. Theorem 1 below is a computationally efficient corollary of the Poincaré-Miranda theorem [4].

Definition 2. Define $\mathbf{x}^{(i-)} \in \mathbb{IR}^n$ and $\mathbf{x}^{(i+)} \in \mathbb{IR}^n$ as follows: $\mathbf{x}_k^{(i\pm)} = \mathbf{x}_k$ for $k \neq i$ and either $\mathbf{x}_i^{(i-)} = \inf \mathbf{x}_i$ or $\mathbf{x}_i^{(i+)} = \sup \mathbf{x}_i$ for $k = i$.

So, $\mathbf{x}^{(i\pm)}$ is a pair of opposite faces of interval box \mathbf{x} .

¹A scanned version of [23] is available at <http://www.goldsztejn.com/downloads.htm>

Theorem 1. Let $\mathbf{x} \in \mathbb{IR}^n$ be an interval vector and $f : \mathbf{x} \longrightarrow \mathbb{R}^n$ be a continuous function. Consider a real vector $\tilde{x} \in \mathbf{x}$. Let $\mathbf{J} \in \mathbb{IR}^{n \times n}$ be a LIM for f and \mathbf{x} . Suppose that $\forall i \in [1..n]$ both

$$\sup(f_i(\tilde{x}) + \mathbf{J}_{i:} \cdot (\mathbf{x}^{(i-)} - \tilde{x})) \leq 0 \quad (5)$$

and

$$0 \leq \inf(f_i(\tilde{x}) + \mathbf{J}_{i:} \cdot (\mathbf{x}^{(i+)} - \tilde{x})), \quad (6)$$

where $\mathbf{J}_{i:} \in \mathbb{IR}^{1 \times n}$ is the i^{th} row of \mathbf{J} . Then there exists $x \in \mathbf{x}$ such that $f(x) = 0$.

The following definition allows Theorem 1 to be conveniently reformulated to aid the forthcoming Corollary 1.

Definition 3. Let $\mathbf{x}, \mathbf{z} \in \mathbb{IR}^n$, $\tilde{x} \in \mathbf{x}$ and $\mathbf{J} \in \mathbb{IR}^{n \times n}$ and for $i \in \{1, \dots, n\}$ define the reals

$$\underline{\mathbf{b}}_i := \sup(\mathbf{z}_i + \mathbf{J}_{i:} \cdot (\mathbf{x}^{(i-)} - \tilde{x})) \quad (7)$$

$$\overline{\mathbf{b}}_i := \inf(\mathbf{z}_i + \mathbf{J}_{i:} \cdot (\mathbf{x}^{(i+)} - \tilde{x})). \quad (8)$$

Define, $\mathcal{I}(\mathbf{x}, \tilde{x}, \mathbf{z}, \mathbf{J})$ and $\mathcal{O}(\mathbf{x}, \tilde{x}, \mathbf{z}, \mathbf{J})$ in the following way: if $\underline{\mathbf{b}}_i \leq \overline{\mathbf{b}}_i$ holds for all $i \in [1..n]$ then $\mathcal{I}(\mathbf{x}, \tilde{x}, \mathbf{z}, \mathbf{J}) := \mathbf{b}$ (where $\mathbf{b}_i = [\underline{\mathbf{b}}_i, \overline{\mathbf{b}}_i]$). Otherwise $\mathcal{I}(\mathbf{x}, \tilde{x}, \mathbf{z}, \mathbf{J}) := \emptyset$. While, $\mathcal{O}(\mathbf{x}, \tilde{x}, \mathbf{z}, \mathbf{J}) := \mathbf{z} + \mathbf{J}(\mathbf{x} - \tilde{x})$.

Then Theorem 1 can be stated in the following way: using the notations introduced in Theorem 1, if $0 \in \mathcal{I}(\mathbf{x}, \tilde{x}, \mathbf{z}, \mathbf{J})$ then there exists $x \in \mathbf{x}$ such that $f(x) = 0$. The following corollary of Theorem 1 allows one to build inner approximations of the image of \mathbf{x} by f . Outer approximation is also considered in Corollary 1 for an homogenized presentation.

Corollary 1. Let $\mathbf{x} \in \mathbb{IR}^n$ be an interval vector and $f : \mathbf{x} \longrightarrow \mathbb{R}^n$ be a continuous function. Consider a real vector $\tilde{x} \in \mathbf{x}$ and an interval vector $\mathbf{z} \in \mathbb{IR}^n$ that contains $f(\tilde{x})$. Let $\mathbf{J} \in \mathbb{IR}^{n \times n}$ be a LIM for f and \mathbf{x} . Then

$$\mathcal{I}(\mathbf{x}, \tilde{x}, \mathbf{z}, \mathbf{J}) \subseteq \text{Range}(f, \mathbf{x}) \subseteq \mathcal{O}(\mathbf{x}, \tilde{x}, \mathbf{z}, \mathbf{J}). \quad (9)$$

Proof. The second inclusion is obvious. Now consider the first inclusion. If the $\mathcal{I}(\mathbf{x}, \tilde{x}, \mathbf{z}, \mathbf{J})$ is empty then the first inclusion trivially holds. Now suppose that the $\mathcal{I}(\mathbf{x}, \tilde{x}, \mathbf{z}, \mathbf{J})$ is not empty and consider any fixed $z \in \mathcal{I}(\mathbf{x}, \tilde{x}, \mathbf{z}, \mathbf{J})$ and define the auxiliary function $g(x) := f(x) - z$. We just have to prove that g has a zero in \mathbf{x} . The interval matrix \mathbf{J} is obviously also a LIM for g and \mathbf{x} . By definition of $\mathcal{I}(\mathbf{x}, \tilde{x}, \mathbf{z}, \mathbf{J})$ the following two inequalities hold $\forall i \in [1..n]$:

$$\begin{aligned} \sup(\mathbf{z}_i + \mathbf{J}_{i:} \cdot (\mathbf{x}^{(i-)} - \tilde{x})) \\ \leq z_i \leq \\ \inf(\mathbf{z}_i + \mathbf{J}_{i:} \cdot (\mathbf{x}^{(i+)} - \tilde{x})). \end{aligned} \quad (10)$$

Because $f_i(\tilde{x}) \in \mathbf{z}_i$, we have $\inf \mathbf{z}_i \leq f_i(\tilde{x}) \leq \sup \mathbf{z}_i$ and therefore:

$$\begin{aligned} & \sup(f_i(\tilde{x}) + \mathbf{J}_{i:} \cdot (\mathbf{x}^{(i-)} - \tilde{x})) \\ & \leq z_i \leq \\ & \inf(f_i(\tilde{x}) + \mathbf{J}_{i:} \cdot (\mathbf{x}^{(i+)} - \tilde{x})). \end{aligned} \quad (11)$$

Subtracting the fixed number z_i and noticing that $f_i(x) - z_i = g_i(x)$ we obtain

$$\begin{aligned} & \sup(g_i(\tilde{x}) + \mathbf{J}_{i:} \cdot (\mathbf{x}^{(i-)} - \tilde{x})) \\ & \leq 0 \leq \\ & \inf(g_i(\tilde{x}) + \mathbf{J}_{i:} \cdot (\mathbf{x}^{(i+)} - \tilde{x})). \end{aligned} \quad (12)$$

As this holds for all $i \in [1..n]$, we can apply Theorem 1 so that g has a zero in \mathbf{x} , which concludes the proof. \square

It is worth stressing that the rigorous outer rounding for interval arithmetic leads to rigorous inner approximation thanks to Theorem 1. The $\mathcal{I}(\mathbf{x}, \tilde{x}, \mathbf{z}, \mathbf{J})$ can be nonempty only if the interval matrix \mathbf{J} is close enough to the identity matrix. Formally, \mathbf{J} has to be an interval H-matrix (i.e. contains only H-matrices) as proved in [5]. This is very restrictive and preconditioning is the usual way to weaken this restrictive necessary condition. The next section shows how the preconditioning usually associated to Theorem 1 leads to parallelepiped approximations when Corollary 1 is used.

3.2 Parallelepiped Approximations

Throughout the section, we consider a function $\phi : \mathbb{R}^n \rightarrow \mathbb{R}^n$ and a set \mathbb{Y}_0 wrapped between two parallelepipeds $\mathbb{A}_0 := \{M_0 u \mid u \in \mathbf{a}_0\}$ and $\mathbb{B}_0 := \{M_0 u \mid u \in \mathbf{b}_0\}$ where $\mathbf{a}_0, \mathbf{b}_0 \in \mathbb{R}^n$ and $M \in \mathbb{R}^{n \times n}$ (i.e. $\mathbb{A}_0 \subseteq \mathbb{Y}_0 \subseteq \mathbb{B}_0$). We aim to construct two parallelepipeds $\mathbb{A}_1 := \{M_1 u \mid u \in \mathbf{a}_1\}$ and $\mathbb{B}_1 := \{M_1 u \mid u \in \mathbf{b}_1\}$ such that

$$\mathbb{A}_1 \subseteq \mathbb{Y}_1 \subseteq \mathbb{B}_1 \text{ where } \mathbb{Y}_1 := \text{Range}(\phi, \mathbb{Y}_0). \quad (13)$$

We require the parallelepiped characteristic matrices M_0 and M_1 to be nonsingular. The actual description of \mathbb{Y}_0 being the wrapping parallelepipeds \mathbb{A}_0 and \mathbb{B}_0 , we are going to compute \mathbb{A}_1 and \mathbb{B}_1 such that

$$\mathbb{A}_1 \subseteq \text{Range}(\phi, \mathbb{A}_0) \text{ and } \text{Range}(\phi, \mathbb{B}_0) \subseteq \mathbb{B}_1, \quad (14)$$

which obviously implies (13). In order to apply Corollary 1, we need to work in some auxiliary bases where parallelepipeds will be represented by their characteristic boxes. This is represented in the following diagram where the left hand side represents the actual action of ϕ , and the right hand side represents the action of ϕ in the auxiliary bases, leading to the function $\psi := M_1^{-1} \circ \phi \circ M_0$ (matrices are

identified to the linear mappings they represent).

$$\begin{array}{ccc} \mathbb{A}_0 \subseteq \mathbb{Y}_0 \subseteq \mathbb{B}_0 & \xleftarrow{M_0} & \mathbf{a}_0 \subseteq \tilde{\mathbb{Y}}_0 \subseteq \mathbf{b}_0 \\ \downarrow \phi & & \downarrow \psi \\ \mathbb{A}_1 \subseteq \mathbb{Y}_1 \subseteq \mathbb{B}_1 & \xleftarrow{M_1} & \mathbf{a}_1 \subseteq \tilde{\mathbb{Y}}_1 \subseteq \mathbf{b}_1 \end{array}$$

In the auxiliary bases, we have $\mathbf{a}_0 \subseteq \tilde{\mathbb{Y}}_0 \subseteq \mathbf{b}_0$, where $\tilde{\mathbb{Y}}_0 := \{M_0^{-1} y \mid y \in \mathbb{Y}_0\}$, and we need to construct \mathbf{a}_1 and \mathbf{b}_1 such that $\mathbf{a}_1 \subseteq \tilde{\mathbb{Y}}_1 \subseteq \mathbf{b}_1$, where $\tilde{\mathbb{Y}}_1 := \text{Range}(\psi, \tilde{\mathbb{Y}}_0)$. So we can use Corollary 1 and obtain \mathbf{a}_1 and \mathbf{b}_1 such that

$$\mathbf{a}_1 \subseteq \text{Range}(\psi, \mathbf{a}_0) \subseteq \tilde{\mathbb{Y}}_1 \subseteq \text{Range}(\psi, \mathbf{b}_0) \subseteq \mathbf{b}_1, \quad (15)$$

Therefore, coming back in the original basis (through M_1) they give rise to the inner and outer approximations \mathbb{A}_1 and \mathbb{B}_1 that satisfy (14) and eventually (13). The matrix M_1 , which gives the parallelepiped \mathbb{A}_1 and \mathbb{B}_1 their shape, can be chosen arbitrarily. Some possible choices are proposed in Subsection 3.3.

In order to apply Corollary 1 with the function ψ , we need a LIM for this function and \mathbf{b}_0 . The next proposition aids the computation of such a LIM.

Proposition 1. *Let \mathbf{J} be a LIM for $\phi : \mathbb{R}^n \rightarrow \mathbb{R}^n$ and $\mathbb{B} := \{Mu \mid u \in \mathbf{b}\}$, where $M \in \mathbb{R}^{n \times n}$ and $\mathbf{b} \in \mathbb{R}^n$. Consider $M' \in \mathbb{R}^{n \times n}$. Then, $\mathbf{J}' := M' \cdot \mathbf{J} \cdot M$ is a LIM for $\psi := M' \circ \phi \circ M$ and \mathbf{b} .*

Proof. For any $u, v \in \mathbf{b}$, we have $\psi(u) - \psi(v) = M' \phi(Mu) - M' \phi(Mv) = M' (\phi(Mu) - \phi(Mv))$. Now, both $Mu, Mv \in \mathbb{B}$ and \mathbf{J} is a LIM for ϕ and \mathbb{B} , so there exists $J \in \mathbf{J}$ such that $\phi(Mu) - \phi(Mv) = J(Mu - Mv)$. Therefore $\psi(u) - \psi(v) = M' J(Mu - Mv) = M' JM(u - v)$. Finally, as $\mathbf{J}' \supseteq \{M' JM \mid J \in \mathbf{J}\}$, we can find $\tilde{J} \in \mathbf{J}'$ such that $\psi(u) - \psi(v) = \tilde{J}(u - v)$, so \mathbf{J}' is a LIM for ψ and \mathbf{b} . \square

The construction of the parallelepiped inner and outer approximations is formalized by the following theorem.

Theorem 2. *With the notations defined at the beginning of the section, consider $a \in \mathbf{a}_0$ and $b \in \mathbf{b}_0$ and define*

$$\mathbf{a}_1 := \mathcal{I}(\mathbf{a}_0, a, \Psi_a, \mathbf{J}') \quad (16)$$

$$\mathbf{b}_1 := \mathcal{O}(\mathbf{b}_0, b, \Psi_b, \mathbf{J}'), \quad (17)$$

with $\mathbf{J}' := M_1^{-1} \mathbf{J} M_0$ where \mathbf{J} is a LIM for ϕ and \mathbb{B}_0 , and Ψ_a and Ψ_b are interval vectors that contain respectively $\psi(a)$ and $\psi(b)$ with $\psi := M_1^{-1} \circ \phi \circ M_0$. Then

$$\mathbb{A}_1 \subseteq \text{Range}(\phi, \mathbb{Y}_0) \subseteq \mathbb{B}_1. \quad (18)$$

Proof. Proposition 1 proves that \mathbf{J}' is a LIM for ψ and \mathbf{b}_0 (and therefore also for ψ and \mathbf{a}_0 because $\mathbf{a}_0 \subseteq \mathbf{b}_0$). From the definitions of \mathbf{a}_1 and \mathbf{b}_1 , we can apply Corollary 1 which proves

$$\mathbf{a}_1 \subseteq \text{Range}(\psi, \mathbf{a}_0) \text{ and } \text{Range}(\psi, \mathbf{b}_0) \subseteq \mathbf{b}_1. \quad (19)$$

By definition of ψ , we have both $\text{Range}(\psi, \mathbf{a}_0) = \text{Range}(M_1^{-1}\phi, \mathbb{A}_0)$ and $\text{Range}(\psi, \mathbf{b}_0) = \text{Range}(M_1^{-1}\phi, \mathbb{B}_0)$. Therefore, applying the linear mapping M_1 to each inclusion (19), we obtain $\mathbb{A}_1 \subseteq \text{Range}(\phi, \mathbb{A}_0)$ and $\text{Range}(\phi, \mathbb{B}_0) \subseteq \mathbb{B}_1$, which concludes the proof by (14). \square

All one needs in order to apply Theorem 2 is:

- (i) Interval enclosures Ψ_a and Ψ_b of $\psi(a)$ and $\psi(b)$. In general, it will be easy to compute some interval enclosures Φ_a and Φ_b of $\phi(M_0a)$ and $\phi(M_0b)$. Then one can use $\Psi_a := M_1^{-1}\Phi_a$ and $\Psi_b := M_1^{-1}\Phi_b$.
- (ii) A LIM \mathbf{J} for ϕ and \mathbb{B}_0 . It will be easier to compute a LIM \mathbf{J} for ϕ and $M_0\mathbf{b}_0$ (the interval vector $M_0\mathbf{b}_0$ being the smallest interval vector that contains \mathbb{B}_0 so $\mathbb{B}_0 \subseteq M_0\mathbf{b}_0$).

In the case where $\phi = \phi_K \circ \dots \circ \phi_2 \circ \phi_1$, Theorem 2 can be applied inductively in the following way: let \mathbb{A}_k and \mathbb{B}_k be respectively inner and outer approximations of the image of \mathbb{Y}_0 by the function $\phi_k \circ \dots \circ \phi_2 \circ \phi_1$, with $k < K$. Then knowing \mathbb{A}_k and \mathbb{B}_k we can compute \mathbb{A}_{k+1} and \mathbb{B}_{k+1} using Theorem 2. This process obviously preserves the interpretations of the approximations, hence leading to $\mathbb{A}_K \subseteq \text{Range}(\phi_K \circ \dots \circ \phi_2 \circ \phi_1, \mathbb{Y}_0) \subseteq \mathbb{B}_K$.

Remark 1. In the case where $\mathbb{A}_{t_k} = \emptyset$ for some $k \in [1..K]$ then $\mathbb{A}_{t_k} = \emptyset$ for $k \in [k..K]$. So, only the outer approximation component of Theorem 2 is used.

3.3 On the Choice of the Parallelepiped Characteristic Matrix

The characteristic matrix M_1 gives their shape to the parallelepiped approximations \mathbb{A}_1 and \mathbb{B}_1 . It can be chosen arbitrarily. However, this choice will decide the quality of the approximations.

As mentioned at the end of Subsection 3.1, $\mathcal{I}(\mathbf{x}, \tilde{x}, \mathbf{z}, \mathbf{J})$ can be nonempty only if \mathbf{J} is an interval H-matrix. The LIM of ψ that will be used is $M_1^{-1}(\mathbf{J}M_0)$. As a consequence of the theory of strongly regular interval matrices [20], $\mathbf{J}M_0$ has to be strongly regular and one should choose $M_1 = \text{mid}(\mathbf{J}M_0)$. This relates in an interesting way the midpoint inverse preconditioning usually used with Theorem 1 to the shape of the parallelogram inner approximation that can be built using Corollary 1.

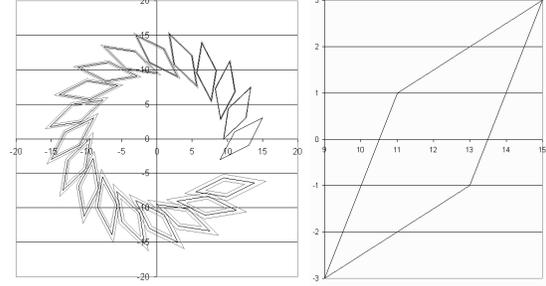


Figure 1.

Finally, if $\mathbf{J}M_0$ is not strongly regular, then no inner approximation is possible. If an outer approximation has to be computed, then $M_1 = \text{mid}(\mathbf{J}M_0)$ may not be an appropriate choice and outer approximation certainly needs a better choice for the auxiliary basis M_1 . In this case, the QR-factorization method, widely used in the context of ordinary differential equation solving, can be used for a better choice of M_1 [24, 19].

3.4 A Linear Mapping Example

Consider the rotation $f(x) = R_\theta x$ where R_θ is the angle θ rotation matrix. We choose $\theta = \pi/10$. We use two Lipschitz interval matrices. The first is obtained by evaluating the derivative of f with interval arithmetic:

$$\mathbf{J} := \begin{pmatrix} 0.95105651629515_3^4 & -0.30901699437494_8^7 \\ 0.30901699437494_8^8 & 0.95105651629515_3^4 \end{pmatrix}, \quad (20)$$

The second, denoted by \mathbf{J}' , is obtained by adding $[-0.001, 0.001]$ to each entry of \mathbf{J} . The choice of the characteristic matrix M_1 is done as proposed in the previous subsection, i.e. $M_1 = \text{mid}(\mathbf{J}M_0)$. The initial parallelepipeds \mathbb{A}_0 and \mathbb{B}_0 are equal to $\{Mx | x \in \mathbf{x}\}$ with

$$M := \begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix} \text{ and } \mathbf{x} := \begin{pmatrix} [7, 9] \\ [-5, -3] \end{pmatrix}. \quad (21)$$

The parallelepiped approximations for the first 18 steps are displayed on the left hand side graphic of Figure 1. Black parallelepipeds are computed using \mathbf{J} . Inner and outer approximations are too close to be distinguishable. Grey parallelepipeds are computed using \mathbf{J}' . This time, due to the poor quality of the LIM, inner and outer approximations quickly separate.

After $K := 10^7$ iterations, i.e. after 5×10^5 complete rotations, the parallelepiped approximations computed using \mathbf{J} are plotted on the right hand side of Figure 1. They are still not distinguishable, and on the scale of the figure the distance between them is less than 10^{-6} .

4 Inner and Outer Approximations of the Solutions to Uncertain Initial Value Problems

The initial value problem (IVP) consists of computing an approximation of the solution to some ordinary differential equation (ODE) for some initial value. The solution at time t can be expressed naturally as a function of the initial value, function called the ODE *solution operator* (cf. subsection 4.1). So when one deals with a set of initial conditions, one needs to approximate the image of a set by the ODE solution operator. The results stated in the previous section can then be used, leading in particular to rigorous inner approximations. Up to our knowledge, the only work that proposes to compute such inner approximations is [14]. However, inner approximation is just mentioned in [14] and no detail can be found on the way such inner approximations can be computed.

4.1 General Framework

IVP with sets of initial values are defined as in [18]. First, given a function $f : \mathbb{R}^n \rightarrow \mathbb{R}^n$ and a vector $y_0 \in \mathbb{R}^n$, the IVP consists of computing a function y that satisfies

$$y'(t) = f(y(t)), \quad (22)$$

$$y(0) = y_0 \in \mathbb{R}^n. \quad (23)$$

The function f is supposed N times continuously differentiable, with $N \geq 1$. In practice, one wishes to compute an approximation of $y(h)$ for a given time-step $h > 0$.

Remark 2. Here, we do not consider explicitly the construction of a solution step-after-step but instead focus one single step. The composition of several steps can be done applying the method described at the end of Subsection 3.2.

Equation (22) is called the *defining equation*, and (23) the *initial value*. To simplify the presentation, we assume existence and uniqueness of the solution to (22) for all initial conditions. It is convenient to describe the solution of the initial value problems with respect to the initial condition using a function $\phi_h : \mathbb{R}^n \rightarrow \mathbb{R}^n$ such that $y(t+h) = \phi_h(y(t))$. This mapping is well defined in \mathbb{R}^n because we assumed existence and uniqueness of the solution to (22). The function ϕ_h is called the *time- h solution operator* of the ODE (22). Thanks to the definition of the ODE solution operator, the IVP problem can be cast into the problem that consists of computing some approximation of $\phi_h(y_0)$.

We now consider a set of initial conditions \mathbb{Y}_0 , called an uncertain initial condition, and (23) is replaced by

$$y(0) \in \mathbb{Y}_0 \subseteq \mathbb{R}^n. \quad (24)$$

We aim to construct some approximation of

$$\mathbb{Y}_h := \{y(h) \mid y \text{ satisfies (22) and (24)}\} \quad (25)$$

$$= \text{Range}(\phi_h, \mathbb{Y}_0). \quad (26)$$

We call this problem an uncertain initial value problem (UIVP). In practice, we suppose that \mathbb{Y}_0 is approximated by an inner and an outer parallelepiped, i.e. $\mathbb{A}_0 \subseteq \mathbb{Y}_0 \subseteq \mathbb{B}_0$ where $\mathbb{A}_0 := \{Uu \mid u \in \mathbf{a}_0\}$ and $\mathbb{B}_0 := \{Uu \mid u \in \mathbf{b}_0\}$. Then, we aim to construct two parallelepipeds $\mathbb{A}_h := \{Vv \mid v \in \mathbf{a}_h\}$ and $\mathbb{B}_h := \{Vv \mid v \in \mathbf{b}_h\}$ such that $\mathbb{A}_h \subseteq \mathbb{Y}_h \subseteq \mathbb{B}_h$. Such approximations can be computed applying Theorem 2 in order to construct inner and outer approximations of $\text{Range}(\phi_h, \mathbb{Y}_0)$. Therefore, all we need are:

- (i) An outer approximation \mathbf{z} of $\phi_h(y_0)$.
- (ii) A LIM of ϕ_h and \mathbb{Y}_0 .

In order to compute (i), one can use the usual interval methods for computing enclosing approximation of IVP. In order to obtain (ii), an enclosure of the derivatives of the solution operator can be computed. Its computation can be expressed as a $n^2 + n$ components IVP. Therefore, the same interval methods can also be used to compute (ii). However, $n^2 + n$ quickly becomes too big for a direct use of interval IVP solvers (which uses the derivatives of the ODE to be integrated, hence leading to $O(n^4)$ Taylor coefficients to be evaluated in this case). The next subsection provide direct methods to compute a LIM for the ODE solution operator.

4.2 Lipschitz Interval Matrices for the ODE Solution Operator

This subsection presents some techniques to compute a LIM for ϕ_h and \mathbb{Y}_0 . Throughout the subsection, we consider two boxes \mathbf{y}_0 and $\mathbf{y}_{[0,h]}$ that contains respectively \mathbb{Y}_0 and $\mathbb{Y}_{[0,t]}$, i.e. \mathbf{y}_0 contains all initial conditions and $\mathbf{y}_{[0,h]}$ contains all trajectories for $t \in [0, h]$ and for any initial condition in \mathbf{y}_0 . While $\mathbf{y}_0 := M_0 \mathbf{b}_0$ is the optimal choice, the computation of $\mathbf{y}_{[0,h]}$ can be more problematic. For small enough time-step h , $\mathbf{y}_{[0,h]}$ can be computed using a rigorous first order approximation: it is indeed sufficient that $\mathbf{y}_{[0,h]}$ satisfies $\mathbf{y}_0 + h f(\mathbf{y}_{[0,h]}) \subseteq \mathbf{y}_{[0,h]}$ so that the Picard-Lindelöf operator proves existence and uniqueness of the solution inside $\mathbf{y}_{[0,h]}$ for any initial value in \mathbf{y}_0 (see e.g. Section 5 in [18]). Higher order and more efficient methods can also be used to compute $\mathbf{y}_{[0,h]}$.

4.2.1 Lipschitz Interval Matrices for Linear ODE

We first consider the case of linear ODE, i.e. $f(y) = Ay$ with $A \in \mathbb{R}^{n \times n}$. It is well known that in this case $\phi_h(y_0) = e^{hA} y_0$. Therefore a LIM for ϕ_h is easily obtained:

Theorem 3. Any interval matrix $\mathbf{J} \in \mathbb{IR}^{n \times n}$ that contains e^{hA} is a LIM for ϕ_h and \mathbb{R}^n .

Proof. Consider any $x, y \in \mathbb{R}^n$. The $\phi_h(y) - \phi_h(x) = e^{hA}y - e^{hA}x$ which is equal to $e^{hA}(y - x)$. Because $e^{hA} \in \mathbf{J}$ by hypothesis, we have eventually $\phi_h(y) - \phi_h(x) \in \mathbf{J}(y - x)$. \square

Remark 3. An interval matrix \mathbf{J} that contains e^{hA} can be constructed following [21] (that uses a truncated Taylor expansion with some specific Householder norms for an accurate computation of the remainder) or [2] (that uses Padé approximations).

Example 1. We consider the linear ODE defined by

$$y'(t) = Ay(t) \text{ with } A = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}. \quad (27)$$

Following the example presented in Subsection 3.4, we fix $h = \frac{\pi}{10}$. Using some rigorous interval approximation of $e^{\frac{\pi}{10}A}$ we obtain a LIM very close to (20). Using an initial condition $y(0) \in \{Mx \mid x \in \mathbf{x}\}$ with (21), the parallelepiped approximations are also similar to the one plotted in the left hand side of Figure 1.

4.2.2 Lipschitz Interval Matrices for Nonlinear ODE

In this section, some enclosures of the derivative of the solution operator w.r.t. the initial condition are computed instead of some LIM (the solution operator is actually differentiable w.r.t. the initial condition, cf. Theorem 14.3 in [7]). Let us recall that $\frac{\partial \phi_t(x)}{\partial x} \Big|_y$ and $\frac{\partial f(x)}{\partial x} \Big|_y$ are denoted by $\phi'_t(y)$ and $f'(y)$ respectively (no confusion will be possible because $\phi_t(y)$ will not be differentiated w.r.t. time). The following theorem can be found e.g. in [3]. It will provide us with a first enclosure of the derivative of the solution operator.

Theorem 4. If $y(t)$ and $z(t)$ each satisfy the differential equation $y'(t) = f(y(t))$ on $[t_0, t_1]$, and f is Lipschitz continuous with constant L , then $\forall t \in [t_0, t_1]$,

$$\|y(t) - z(t)\| \leq \|y(t_0) - z(t_0)\| e^{L(t_1 - t_0)}. \quad (28)$$

Remark 4. As both $y(t) \in \mathbf{y}_{[0, h]}$ and $z(t) \in \mathbf{y}_{[0, h]}$ for any $t \in [0, h]$, a Lipschitz constant for the restriction of f to $\mathbf{y}_{[0, h]}$ can be used in Theorem 4. As a consequence, one can use $L = \|\mathbf{f}'(\mathbf{y}_{[0, h]})\|$.

The next corollary of Theorem 4 provides a crude enclosure of the derivative of the solution operator. It will not be used in practice, but it will be the basis to construct other more accurate enclosures.

Corollary 2. Suppose that f is Lipschitz continuous with constant L inside $\mathbf{y}_{[0, t]}$ and define the interval matrix $\mathbf{J}_{[0, t]}$ by $(\mathbf{J}_{[0, t]})_{ij} := [-e^{hL}, e^{hL}]$. Then, $\mathbf{J}_{[0, t]} \supseteq \{\phi'_t(y_0) \mid y_0 \in \mathbf{y}_0\}$ for all $t \in [0, h]$.

Sketch of the proof. Throughout the proof ϕ_t is simply denoted by ϕ . By definition $\phi'(y_0)$ satisfies $\phi(y_0 + \epsilon\delta) - \phi(y_0) = \epsilon\phi'(y_0) \cdot \delta + \gamma O(\epsilon^2)$, where $\delta, \gamma \in \mathbb{R}^n$ are of norm 1 and $\mathbb{R} \ni \epsilon > 0$. Choose $\delta = e_j$, where e_j is the j^{th} base vector and note that $(\phi'(y_0) \cdot e_j)_i = \phi'_{ij}(y_0)$. One obtains $\phi_i(y_0 + \epsilon e_j) - \phi_i(y_0) = \epsilon\phi'_{ij}(y_0) + O(\epsilon^2)$. As a consequence, $|\phi_i(y_0 + \epsilon e_j) - \phi_i(y_0)| = \epsilon|\phi'_{ij}(y_0)| + O(\epsilon^2)$, which obviously contradicts (28) if $|\phi'_{ij}(y_0)| > e^{tL}$. Therefore, $\phi'_{ij}(y_0)$ has to satisfy $|\phi'_{ij}(y_0)| \leq e^{tL} \leq e^{hL}$. \square

In order to obtain a better enclosure of the derivatives of ϕ , Taylor expansions of ϕ_t and ϕ'_t w.r.t. time are now considered. To this end, the auxiliary functions $y^{[k]}(x)$ are introduced: as f is N times continuously differentiable, $y(t)$ is $N + 1$ times continuously differentiable and $y^{(k)}(t)$, for $k \in [1..N + 1]$, can be computed as a function of $y(t)$. For example in dimension one, $y'(t) = f(y(t))$, $y''(t) = f'(y(t))f(y(t))$, $y^{(3)}(t) = f''(y(t))f(y(t))^2 + f'(y(t))^2f(y(t))$, etc. In order to easily manipulate these expressions, we define $y^{[k]}(x)$ such that

$$y^{[k]}(y(t)) = y^{(k)}(t), \quad (29)$$

with by convention $y^{[0]}(y(t)) = y(t)$. So we have e.g. $y^{[1]}(x) = f(x)$, $y^{[2]}(x) = f'(x) \cdot f(x)$, $y^{[3]}(x) = f''(x)f(x)^2 + f'(x)^2f(x)$, etc. As f is supposed N times continuously differentiable, $y^{[k]}$ is well defined and continuously differentiable for $k \in [1..N]$. The functions $y^{[k]}$ can be evaluated either formally computing their expressions or using automatic differentiation (see e.g. [24, 18]). Then, Taylor's theorem can be written

$$\phi_h(y_0) = \sum_{k=0}^{N-1} \frac{h^k}{k!} y^{[k]}(y_0) + \frac{h^N}{N!} y^{[N]}(\bar{y}_\xi(y_0)), \quad (30)$$

where $y^{[N]}(\bar{y}_\xi(y_0))$ is a non-standard notation to shortly display that each component of $y^{[N]}$ is evaluated for a different $y_\xi \in [0, h]$, each y_ξ depending on y_0 .

Remark 5. The functions $f^{[k]}(x) := \frac{1}{k!} y^{[k]}(x)$ instead of $y^{[k]}(x)$ are defined in [18]. Including $\frac{1}{k!}$ in the expressions is important in implementations as it usually allows stabilizing the recursive evaluation of the expressions while slightly reducing the computational cost of the evaluation.

The next theorem provides a way to improve the first enclosure computed, thanks to Corollary 2.

Theorem 5. Let $\mathbf{J}_{[0, h]}$ be an enclosure of $\{\phi'_t(y_0) \mid y_0 \in \mathbf{y}_0\}$ for all $t \in [0, h]$. Then,

$$\sum_{k=0}^{N-1} \frac{h^k}{k!} \frac{\partial y^{[k]}(x)}{\partial x} \Big|_{\mathbf{y}_0} + \frac{h^N}{N!} \frac{\partial y^{[N]}(x)}{\partial x} \Big|_{\mathbf{y}_{[0, h]}} \cdot \mathbf{J}_{[0, h]} \quad (31)$$

is an enclosure of $\{\phi'_h(x) \mid x \in \mathbf{y}_0\}$.

Proof. Differentiating (30) w.r.t. y_0 and using the chain rule give rise to the following expression for $\phi'_h(y_0)$:

$$\sum_{k=0}^{N-1} \frac{h^k}{k!} \frac{\partial y^{[k]}(x)}{\partial x} \Big|_{y_0} + \frac{h^N}{N!} \frac{\partial y^{[N]}(x)}{\partial x} \Big|_{\vec{y}_\xi(y_0)} \cdot \frac{\partial \vec{y}_\xi(x)}{\partial x} \Big|_{y_0} \quad (32)$$

It remains to note that $y_\xi(y_0) = \phi_\xi(y_0)$ and hence $\frac{\partial \vec{y}_\xi}{\partial x}(y_0) \in \mathbf{J}_{[0,h]}$ while $\vec{y}_\xi(y_0) \in \mathbf{y}_{[0,h]}$ and $y_0 \in \mathbf{y}_0$ to conclude the proof. \square

Remark 6. As for evaluating $y^{[k]}$, evaluating $\frac{\partial y^{[k]}(x)}{\partial x}$ can be done computing its formal expression or using automatic differentiation (see e.g. [24, 18]).

Remark 7. The interval matrix $\mathbf{J}_{[0,h]}$ needed in Theorem 5 is computed using Corollary 2. It is useful to improve this first crude enclosure by

$$\mathbf{J}_{[0,h]} \leftarrow \left(\sum_{k=0}^{N-1} \frac{[0,h]^k}{k!} \cdot \frac{\partial y^{[k]}(\mathbf{y}_0)}{\partial x} + \frac{[0,h]^N}{N!} \cdot \frac{\partial y^{[N]}(\mathbf{y}_{[0,h]})}{\partial x} \cdot \mathbf{J}_{[0,h]} \right) \cap \mathbf{J}_{[0,h]}, \quad (33)$$

which obviously maintains $\mathbf{J}_{[0,t]} \supseteq \{\phi'_t(y_0) \mid y_0 \in \mathbf{y}_0\}$ for all $t \in [0, h]$ thank to Theorem 5. This can be repeated a couple of times to improve the enclosure.

In the special case of first order (31) is

$$I + hf'(\mathbf{y}_{[0,h]}) \cdot \mathbf{J}_{[0,h]}. \quad (34)$$

For small enough values of h , this simple expression together with the improvement process of Remark 7 can already provide useful enclosures of $\{\phi'_h(x) \mid x \in \mathbf{y}_0\}$. Let us first illustrate Theorem 5 with the special case of linear ODE.

Example 2. Let $f(y) = A \cdot y$. In this case, we have $y(t) = e^{tA} \cdot y_0$ and $y'(t) = A \cdot y(t)$ and $y''(t) = A^2 \cdot y(t)$ and so on. Finally, one proves that $y^{(k)}(t) = A^k \cdot y(t)$ and therefore $y^{[k]}(x) = A^k \cdot x$. As a consequence,

$$\frac{\partial y^{[k]}(x)}{\partial x} = A^k. \quad (35)$$

Formula (31) therefore gives rise to

$$I + \sum_{k=1}^{N-1} \frac{h^k}{k!} A^k + \frac{h^N}{N!} A^N \cdot \mathbf{J}_{[0,h]}, \quad (36)$$

where Corollary 2 allows $(\mathbf{J})_{ij} = [-e^{h\|A\|}, e^{h\|A\|}]$. This can be interpreted as a rigorous truncation of the series e^{hA} .

Example 3. The Lorenz system is defined by

$$\begin{pmatrix} x'(t) \\ y'(t) \\ z'(t) \end{pmatrix} = \begin{pmatrix} \sigma(y(t) - x(t)) \\ x(t)(\rho - z(t)) - y(t) \\ x(t)y(t) - \beta z(t) \end{pmatrix} \quad (37)$$

We use the usual values $\sigma = 10$, $\rho = 28$ and $\beta = 8/3$, for which the system exhibits a chaotic behavior [15]. The uncertain initial condition is chosen to be $\mathbf{y}_0 = (10 \pm 10^{-10}, 10 \pm 10^{-10}, 10 \pm 10^{-10})$. Then applying Theorem 5 with 20^{th} order expansions and a timestep of $h = 0.02$ gives rise to one-timestep distance between the inner and outer approximations of less than 1.5×10^{-4} .

4.2.3 Related Work

Only a very few references deal with the problem of a rigorous computation of a LIM for an ODE solution operator. The parallelepiped method proposed by Kruckeberg in [14] implicitly uses

$$\sum_{k=0}^{\infty} \frac{h^k \mathbf{J}_f^k}{k!}, \quad (38)$$

where $\mathbf{J}_f \supseteq \{f'(x) \mid x \in \mathbf{y}_0\}$, as a LIM for ϕ_h . However the proof of this property is not detailed in [14] (see formula 29 page 95²). And more important, no rigorous truncation of (38) is available. The rigorous truncation proposed in [21] cannot be applied to (38) because $\{\exp(hJ_f) \mid J_f \in \mathbf{J}_f\}$ is not equal to (38), while no simplification (e.g. Horner scheme) can be applied to (38) until one has proved the simplified formula is also a LIM for ϕ_h (i.e. it is likely to happen that the overestimation of $\{\exp(hJ_f) \mid J_f \in \mathbf{J}_f\}$ in the expression (38) is necessary to obtain a LIM).

Stauning [24] proposes (formula 6.17 and 6.18 page 69) the following LIM:

$$I + \sum_{k=1}^{N-1} \frac{1}{k!} \frac{\partial y^{[k]}(\mathbf{y}_0)}{\partial y} h^k + \frac{1}{N!} \frac{\partial y^{[N]}(\mathbf{y}_{[0,h]})}{\partial y} h^N \quad (39)$$

However, Stauning's result is false: (39) is not a LIM for ϕ_h and \mathbf{y}_0 in general (in the case of a linear system, (39) just truncates the series e^{tA} without providing any remainder). The correct formula is the one provided in Theorem 5.

Makino [16] notes that Taylor models cannot help computing a LIM for ϕ_h and just mentions a potential method for the computation of \mathbf{J} (cf. page 92 of [16]).

Finally, the authors have recently discovered the work of Zgliczynski [26] where the derivative of the solution operator is rigorously enclosed. Though both works are similar, our presentation seems simpler while providing some similar enclosures. The exact relationship between the two methods remains to be investigated.

5 Conclusion

While the outer approximation of the range of a function is a basic application of interval analysis, the inner ap-

²A scanned version of [14] is available at <http://www.goldsztein.com/downloads.htm>

proximation of the range remains today a problem not well solved. A new procedure for the computation of such an inner approximation has been proposed, based on a corollary of the Poincaré-Miranda theorem: for roughly no additional cost, one is now able to compute an inner approximation together with the outer approximation given by the mean-value extension. The inner approximation will not be empty only in the situations where the mean-value extension provides a sharp enclosure. In particular, the interval Lipschitz matrix used has to be an H-matrix. A specific preconditioning process has been proposed to help fulfilling this necessary condition, leading to parallelepiped approximations. Due to some potential applications in the theory of shadowing dynamical systems, some properties that allow us to compute Lipschitz interval matrices in the context of ordinary differential equations have been presented.

Experiments are currently underway to apply these developments to the rigorous shadowing of dynamical systems, and in particular the Lorenz system, using ideas similar to those in [9].

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