Interval Superposition Arithmetic for Guaranteed Parameter Estimation

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Abstract: The problem of guaranteed parameter estimation (GPE) consists in enclosing the set of all possible parameter values, such that the model predictions match the corresponding measurements within prescribed error bounds. One of the bottlenecks in GPE algorithms is the construction of enclosures for the image-set of factorable functions. In this paper, we introduce a novel set-based computing method called interval superposition arithmetics (ISA) for the construction of enclosures of such image sets and its use in GPE algorithms. The main benefits of using ISA in the context of GPE lie in the improvement of enclosure accuracy and in the implied reduction of number set-membership tests of the set-inversion algorithm.

Keywords: Set Arithmetics, Interval arithmetics, Guaranteed Parameter Estimation.

1. INTRODUCTION

In science and engineering, the behavior of processes and systems is often described using a mathematical model. Mathematical model development often follows three steps: model structure specification, design (and realization) of experiments, and estimation of unknown model parameters (Franceschini and Macchietto, 2008). In the last step, parameters are sought for which the model outputs match available measurements (Ljung, 1999).

One possible way of addressing the parameter estimation problem is the use of set-membership estimation (Milanese and Vicino, 1991; Bai et al., 1995), also called guaranteed parameter estimation (GPE). The GPE problem can be formulated as an identification of the set of all possible model parameter values which are not falsified by the plant measurements, within some prescribed error bounds. A set-inversion algorithm (e.g. SIVIA by Jaulin and Walter, 1993) can be applied to find such set for nonlinear models. Here, the parameter set is successively partitioned into smaller boxes and using exclusion tests some of these boxes are eliminated, until a desired approximation is achieved. Since its advent, GPE has found various applications (see e.g., Marco et al., 2000; Jaulin et al., 2002; Lin and Stadtherr, 2007; Hast et al., 2015; Paulen et al., 2016).

The complexity of the search procedure in SIVIA is proportional to the tightness of the interval enclosures. Considerable effort has then been invested into developing different set-arithmetics (Makino and Berz, 1996; Paulen et al., 2016, such as Taylor models) to produce tighter enclosures of image-set of nonlinear factorable functions. These techniques usually require computing and storing quantities such as sensitivity information.

Here, we propose an attempt to improve GPE algorithms using a novel non-convex set-arithmetic called Interval Superposition Arithmetic (ISA). This arithmetic operates over Interval Superposition models (ISM), representing a piecewise constant enclosure over a grid of the domain. Unlike a naive application of interval arithmetics (IA) over the grid, the computational and storage complexity of ISA is polynomial. Furthermore, it is able to exploit separable structures in the computational graph of a factorable function. Finally, unlike Taylor model arithmetics—which are based on local information—ISA is based on globally valid algebraic relations. As a result, ISMs are tighter than Taylor models—at least over large domains.

The rest of the paper is organized as follows, Section 2 reviews GPE and set-inversion. Section 3 presents an overview of ISA. An algorithm for intersecting ISMs with an interval—which forms the basis for a set-inversion algorithm—is presented in Section 4. It is important to notice that the intersection algorithm runs in polynomial time, but the complexity of computing an arbitrarily close approximation of the parameter set is exponential. The application of the proposed algorithm to a simple case study is shown in Section 5. Section 6 concludes the paper.

Notation The set of real valued compact interval vectors is denoted by $\mathbb{I}^n = \{ [a, b] \subseteq \mathbb{R}^n | a, b \in \mathbb{R}^n, a \leq b \}$. Let $I = [a, b] \subseteq \mathbb{R}$ and $c \in \mathbb{R}$, $c + I = I + c$ we have $[a + c, b + c]$. Similarly, $cI = Ic$ denotes $[ca, cb]$ if $c \geq 0$ ([cb, ca] if $c < 0$). The diameter of $I$ is denoted by $\text{diam}(I) = b - a$. Interval operations are evaluated by IA (Moore et al., 2009), e.g.,

$[a, b] + [c, d] = [a + c, b + d]$, $[a, b] * [c, d] = \lfloor \min\{ac, ad, bc, bd\} \rfloor$, $\max\{ac, ad, bc, bd\}$

$\exp([a, b]) = \{\exp(a), \exp(b)\}$
2. GUARANTEED PARAMETER ESTIMATION

We consider a system represented by the algebraic model
\[ y = f(x). \]  
(1)
Here, \( x \in \mathbb{R}^n \) denotes unknown parameter while \( y \in \mathbb{R}^m \) the (observed) output variables. The model is described by the, possibly nonlinear, function \( f : \mathbb{R}^n \rightarrow \mathbb{R}^m \).

Given \( n_m \in \mathbb{N} \) measurements, \( y_1^m, \ldots, y_{n_m}^m \in \mathbb{R}^m \), the GPE paradigm works under the assumption that true system outputs \( y_1, \ldots, y_N \) can be observed only within some bounded measurement bounds. Thus, for each \( i \in \{1, \ldots, n_m\} \), we have
\[ y_i^m \in y_i^m + [-\eta_i, \eta_i] =: Y_i \subset \mathbb{R}^m \]  
(2)
with \( \eta_1, \ldots, \eta_{n_m} \geq 0 \). The aim of GPE is to compute the set
\[ X_0 := \{ x \in X_0 \mid \forall i \in \{1, \ldots, N\} : f(x) \in Y_i \} \]  
(3)
i.e., the set of parameters (within some admissible domain \( X_0 \in \mathbb{R}^n \)) for which the model outputs are consistent with all the uncertain observations \( Y_i \).

Computing (3) requires intersecting the preimage of \( Y_i \) under \( f \), with the initial parameter domain, i.e.,
\[ X_e = \left( \bigcap_{i=1}^{n_m} f^{-1}(Y_i) \right) \cap X_0. \]  
(4)
This problem is intractable, in all but the simplest of cases, and thus one has to settle for approximations of this set. State-of-the-art algorithms for set inversion provide inner \( (X_{\text{int}}) \) and boundary \( (X_{\text{bnd}}) \) subpartitions, i.e. lists of non overlapping interval vectors, satisfying
\[ \bigcup_{X \in X_{\text{int}}} X \subseteq X_e \subseteq \left( \bigcup_{X \in X_{\text{int}}} X \right) \cup \left( \bigcup_{X \in X_{\text{bnd}}} X \right). \]  
(5)
In a nutshell, these algorithms work by subdividing the parameter domain \( X_0 \) into smaller boxes such that \( X_0 = \bigcup_j X_j \). Set arithmetics are then used to construct enclosures of \( f \) on \( X_j \), i.e. sets \( \overline{f_j} \subset \mathbb{R}^m \) satisfying
\[ \overline{f_j} \supseteq \{ f(x) \mid x \in X_j \}. \]  
(6)
Using the information provided by the enclosure \( f_j \), the following set membership tests can be performed to classify the parameter boxes \( X_j \) as interior or boundary boxes:

1. If \( \overline{f_j} \subseteq Y_i \) for all \( i \in \{1, \ldots, n_m\} \), \( X_j \in X_{\text{int}} \)
2. Else, if \( Y_i \cap f(X) = \emptyset \) for some \( i \in \{1, \ldots, n_m\} \), \( X_j \cap X_e = \emptyset \)
3. Else, \( X_j \in X_{\text{bnd}} \).

Figure 1 shows the result of the above process for the function \( f = x_1^2 + x_2^2 \) over \( X_0 = [-3, 3]^2 \), with \( Y = [-2, 2] \). The set \( X_0 \) has been divided into \( N = 20 \) equidistant pieces along each coordinate, resulting in 400 interval vectors \( X_j \). The plot shows the set \( \bigcup_{j=1}^{N} (X_j \times \overline{f_j}) \) and its projection onto the \((x_1, x_2)\)-space. The red and blue boxes belong to \( X_{\text{int}} \) and \( X_{\text{bnd}} \) respectively.

In practice, the domain \( X_0 \) is subdivided iteratively by bisecting boundary boxes, starting with \( X_{\text{bnd}} = X_0 \) and \( X_{\text{int}} = \emptyset \). The bounding, set-membership, and bisection operations are repeated until a termination criterion, e.g.
\[ \forall X \in X_{\text{bnd}} : \text{diam}(X) \leq \epsilon, \]  
(7)
for a user-defined tolerance \( \epsilon > 0 \), is met.

One of the bottlenecks of set inversion algorithms is the over-conservatism of existing set-arithmetics, particularly over large domains. Hence we propose to approach this problem within a novel set-arithmetics paradigm.

3. INTERVAL SUPERPOSITION ARITHMETIC

Interval superposition arithmetic is a novel enclosure method for the image set of nonlinear factorable functions. It propagates nonconvex sets, called interval superposition models, through the computational graph of the function. Unlike Taylor (Makino and Berz, 1996) and Chebyshev models (Battles and Trefethen, 2004; Rajyaguru et al., 2017), ISA does not rely on local approximation methods, instead relying on global algebraic properties and partially separable structures within the function.

3.1 Interval superposition models

Consider an interval domain \( X = [x_1, x_1] \times \ldots \times [x_n, x_n] \). Now, take a partition of \( X \) into intervals of the form
\[ X^j_i = [x_i + (j-1)h_i, x_i + jh_i] \quad \text{with} \quad h_i = \frac{x_i - x_i}{N}, \]  
(8)
for all \( i \in \{1, \ldots, n\} \) and all \( j \in \{1, \ldots, N\} \), with \( N \) being a user-specified integer. An interval superposition model of a real-valued function \( f : \mathbb{R}^n \rightarrow \mathbb{R} \) on \( X \) is an interval valued function \( \Gamma : X \times \mathbb{R}^n \rightarrow \mathbb{R} \), given by
\[ \Gamma(x, A, X) = \sum_{j=1}^{N} \sum_{i=1}^{n_x} A^j_i \phi^j_i(x), \]  
(9)
with
\[ \phi^j_i(x) = \begin{cases} 1 & \text{if } x_i \in X^j_i, \\ 0 & \text{otherwise.} \end{cases} \]  
(10)
Here, \( A^j_i = [A^j_i, \overline{f^j_i}] \) are the components of a matrix
\[ A = \begin{pmatrix} A_1^1 & \ldots & A_1^N \\ \vdots & \ddots & \vdots \\ A_n^1 & \ldots & A_n^N \end{pmatrix} \in \mathbb{R}^{n_x \times N}, \]  
(11)
which, for a fixed \( X \), completely determines the enclosure function of \( f \). Note that ISMs for functions \( f : \mathbb{R}^n \rightarrow \mathbb{R}^m \).
are defined by stacking ISMs for each $f_i$. The matrix $A$ is constructed such that $\Gamma(\cdot, A, X)$ is a piecewise constant enclosure function of $f$ over $X$, i.e.

$$\forall x \in X : \quad f(x) \in \Gamma(x, A, X).$$

The name interval superposition is motivated by the structure of the enclosure function: At any $x \in X^1 \times \ldots \times X^N$, the interval $\mathbb{Y} = \Gamma(x, A, X)$ is given by the Minkowski sum (or superposition) of $n_x$ interval functions $\sum_{i=1}^{n_x} A_i \varphi_i(x)$. The separable structure of ISMs allows for a storage complexity of order $O(n_x N)$, since only $n_x N$ intervals need to be stored, in the matrix $A$, to represent the $N^{n_x}$ pieces of the enclosure. In Figure 1 the graph of an ISM, over a partition of $X$ (with $N = 20$) is shown. Although this set consists of 400 interval vectors (shown in red, white and blue), only 40 intervals are stored in the matrix $A$.

This separability also allows for the global minima and maxima of $\Gamma(\cdot, A, X)$ over $X$:

$$\lambda(A) = \min_{i=1}^{n_x} \alpha x \in X : \quad (\alpha \circ g)(x) \in \Gamma(x, A, X).$$

Here, $\alpha \circ g$ denotes the composition of $\alpha$ and $g$.

Bivariate composition rules in ISA are defined analogously, with the map taking both $A$ and $B$ as inputs. Although such maps are specific for each atom operation $\alpha$, the main steps are outlined in Algorithms 1 and 2 for univariate compositions and bivariate products respectively. The addition rule in interval superposition arithmetic is simple. An interval superposition model of $g + h$ on $X$ is parameterized by the matrix $C = A + B$, with the sum computed componentwise using interval arithmetics.

**Theorem 1.** Let $\Gamma(x, A, X)$ and be an ISM of $g$ on $X$. If the matrix $C \in \mathbb{R}^{n_x \times N}$ is computed using Algorithm 1, then $\Gamma(x, C, X)$ is an ISM of $\alpha \circ g$ on $X$.

**Proof.** For any $x \in X$ be an arbitrary point. Since $\Gamma(x, A, X) = \sum_{i=1}^{n_x} \sum_{j=1}^{N} A_i \varphi_j(x)$ is an ISM of $g$, there exists a sequence $j_1, \ldots, j_{n_x} \in \{1, \ldots, N\}$ and points $y_i \in A_i$ satisfying $g(x) = \sum_{i=1}^{n_x} y_i$. Let $\delta_i = y_i - a_i$, with $\omega$ defined as in Algorithm 1 one can write

**Algorithm 1.** Composition rule of interval superposition arithmetic

**Input:** Matrix $A$ parameterizing $F_{\alpha, X}$ and an atom operation $\alpha$.

**Main Steps:**

1. Choose, for all $i \in \{1, \ldots, n_x\}$, central points $a_i \in \mathbb{R}$ satisfying

$$L(A_i) \leq a_i \leq U(A_i)$$

and set $\omega = \sum_{i=1}^{n_x} a_i$.

2. Choose a suitable remainder bound $r_{\alpha}(A) \geq 0$ such that

$$\sum_{i=1}^{n_x} \alpha(\omega + \delta_i) - (n_x - 1) \omega \leq r_{\alpha}(A)$$

for all $\delta \in \mathbb{R}^{n_x}$.

3. Compute the interval valued coefficients $C_{ij} = \alpha(\omega - a_i + A_i^j) - \frac{n_x - 1}{n_x} \omega$.

**Output:** Matrix $C \in \mathbb{R}^{n_x \times N}$ parameterizing $\Gamma(\cdot, C, X)$ for $\alpha \circ g$.

**Algorithm 2.** Product rule of interval superposition arithmetic

**Input:** Matrices $A$ and $B$ parameterizing $F_{g, X}$ and $F_{b, X}$.

**Main Steps:**

1. Compute the central points, $\forall i \in \{1, \ldots, n_x\}$

$$a_i = \frac{U(A_i) + L(A_i)}{2}$$

and $b_i = \frac{U(B_i) + L(B_i)}{2}$

then set

$$a = \sum_{i=1}^{n_x} a_i, \quad b = \sum_{i=1}^{n_x} b_i, \quad c = \sum_{i=1}^{n_x} a_i b_i, \quad \text{and} \quad \omega = \frac{ab - c}{n_x}.$$

2. Compute $\rho_i(A) = \frac{U(\alpha(A_i)) - L(\alpha(A_i))}{2}$ and $\rho_i(B) = \frac{U(\alpha(B_i)) - L(\alpha(B_i))}{2}$ for all $i \in \{1, \ldots, n_x\}$ as well as the associated remainder bound

$$R(A, B) = \sum_{i=1}^{n_x} \rho_i(A) - \sum_{i=1}^{n_x} \rho_i(B) + \rho_i(A) \rho_i(B).$$

3. Compute, for each $i \in \{1, \ldots, n_x\}$ and all $j \in \{1, \ldots, N\}$

$$C_{ij} = (A_i^j + a - a_i) (B_i^j + b - a) - (a - a_i) (b - b_i) - \omega.$$

4. Set $C_{ij} \leftarrow C_{ij} + R(A, B) \cdot [-1, 1]$ for all $j \in \{1, \ldots, N\}$ with

$$k \in \arg \max_{i=1}^{n_x} \sum_{j=1}^{N} C_{ij}^j.$$

**Output:** Matrix $C \in \mathbb{R}^{n_x \times N}$ parameterizing $\Gamma(\cdot, C, X)$, for $g \ast h$. 

$$\alpha(g(x)) = \alpha \left( \omega + \sum_{i=1}^{n_x} \delta_i \right)$$

$$= \sum_{i=1}^{n_x} \sum_{i=1}^{n_x} \left( \alpha(\omega + \delta_i) - (n_x - 1) \omega \alpha \left( \omega + \sum_{i=1}^{n_x} \delta_i \right) \right) \cdot r_{\alpha}(A)[-1, 1].$$
Since $\delta_i \in A_{ij}^k - a_i$, we have $a(\omega - a_i + A_{ij}^k)$ and
\[
\alpha(g(x)) \in \sum_{i=1}^{n_x} \left( a(\omega - a_i + A_{ij}^k) - \frac{n_x - 1}{n_x} a(\omega) \right) + r_\alpha(A)[-1, 1] = \sum_{i=1}^{n_x} c_i^\alpha,
\]
which implies the statement of the theorem. \qed

**Theorem 2.** Let $\Gamma(x, A, X)$ and $\Gamma(x, B, X)$ be ISMs of $g$ and $h$, respectively, on $X$. If $C \in \Gamma_{n_x \times N}$ is computed using Algorithm 2, then $\Gamma(x, C, X)$ is an ISM of $g \ast h$ on $X$.

A proof of Thm. 2 proceeds along the same lines as the proof of Thm. 1 and its omitted for the sake of brevity.

The construction of remainder bounds and central points used in Algorithm 1 exploits globally valid algebraic properties, called addition theorems, of common univariate operations. As an example, for the exponential function, the addition theorems $e^{x+y} = e^x e^y$ and $e^{x+y} + e^{x-y} = e^{2x} e^y$ hold globally over the real numbers. Letting $t_i = e^y - 1$, $r_\alpha(A)$ can be constructed by bounding the left-hand side of the expression in Step 2) of Algorithm 1. This yields the expression
\[
e\left[ n_x \sum_{i=1}^{n_x} t_i + 1 - \prod_{i=1}^{n_x} (1 + t_i) \right] \leq e\left[ n_x \sum_{i=1}^{n_x} (1 + s_i) - \sum_{i=1}^{n_x} s_i - 1 \right]
\]
with $s_i = \max\{e^{U(A_i)} - a_i - 1, 1 - e^{L(A_i)} - a_i\}$. Choosing $a_i = \log\left( \frac{1}{2} \left( e^{U(A_i)} + e^{L(A_i)} \right) \right)$, minimizes $s_i = e^{U(A_i)} - e^{L(A_i)}$.

The technical derivations for the remainder bounds $r_\alpha(A)$ and the central points $a_i$ for other atom operations can be found in (Zha et al., 2016).

The final ingredient for an arithmetic of interval superpositions models is the construction of a (trivial) ISM for the transition models is the construction of a (trivial) ISM for the

This section proposes a novel search strategy based on ISA for addressing GPE. It has as its core computing the intersection of an ISM with an interval.

Consider an ISM, of the function $f$ over $X$, parameterized by $A \in \Gamma_{n_x \times N}$. The direct way of computing the intersection between this ISM and $Y = [y_1, y_2]$ is to compute the value of the ISM at each interval $X_{i_1} \times \cdots \times X_{i_n}$ in the partition of $X$. This requires computing all possible superpositions of coefficients $A_I$. Such approach, while straightforward, is unfortunately not efficient since its computational complexity is $O(N^{n_x})$.

### Algorithm 3. Intersection of a superposition model with an interval

**Input:** Parameters $A$ and $X$ of the input model and an interval $Y$

**Main Step:**

1. Sort each $A_j$ to obtain the permutations $\Pi$ and $\Pi$.
2. Choose a finite number $n_j$ of intervals $I_j = [0, l_j]$ with index vectors $l_j \in \{1, \ldots, n_j\}$ such that
\[
\forall k \in \{1, \ldots, n_j\}, \quad \sum_{i=1}^{n_x} e_i^\Pi(f(l_j)) \leq \gamma
\]
3. Choose a finite number $n_j$ of intervals $J_j = [0, l_j]$ with index vectors $l_j \in \{1, \ldots, n_j\}$ such that
\[
\forall k \in \{1, \ldots, n_j\}, \quad \sum_{i=1}^{n_x} e_i^\Pi(J_j) \geq \gamma
\]
**Output:** Permutations $\Pi$, $\Pi$ and intervals $\mathcal{J} = (\mathcal{J}_1, \ldots, \mathcal{J}_{n_j})$, $\mathcal{J} = (\mathcal{J}_1, \ldots, \mathcal{J}_{n_j})$.

As it turns out, computing an over approximation of the desired interval can be done by testing only certain selected combinations. The proposed approach, requires sorting the components $A_I = [A_I, \overline{A}_I]$ of the rows $A_i$ of the matrix $A$ in both decreasing and increasing orders. The corresponding permutations are denoted by the functions $\pi_i, \overline{\pi}_i : \{1, \ldots, N\} \rightarrow \{1, \ldots, N\}$ satisfying
\[
\overline{A}^{\Pi(1)}_{I_i} \geq \overline{A}^{\Pi(2)}_{I_i} \geq \cdots \geq \overline{A}^{\Pi(N)}_{I_i}
\]
and
\[
\overline{A}^{\Pi(1)}_{I_i} \leq \overline{A}^{\Pi(2)}_{I_i} \leq \cdots \leq \overline{A}^{\Pi(N)}_{I_i}
\]
In the following, we use the shorthand $\Pi = (\pi_1, \ldots, \pi_{n_x})$ and $\overline{\Pi} = (\overline{\pi}_1, \ldots, \overline{\pi}_{n_x})$. The main pre-processing step for computing a set inversion is outlined in Algorithm 3.

**Theorem 3.** Let $\Pi, \overline{\Pi}$ and $\mathcal{J} = (\mathcal{J}_1, \ldots, \mathcal{J}_{n_j})$, $\mathcal{J} = (\mathcal{J}_1, \ldots, \mathcal{J}_{n_j})$ be computed by Algorithm 3. Define
\[
\Xi = \bigcup_{k \in \{1, \ldots, n_j\}} \bigcup_{j \in \mathcal{J}_k} \Xi_{\pi_i}^{\Pi(j_1)} \times \cdots \times \Xi_{\pi_i}^{\Pi(j_n)} (\Xi_{\pi_i}^{\Pi(j_n)}) (\Xi_{\pi_i}^{\Pi(j_1)})\tag{13}
\]
\[
\Xi = \bigcup_{k \in \{1, \ldots, n_j\}} \bigcup_{j \in \mathcal{J}_k} \Xi_{\overline{\pi}_i}^{\Pi(j_1)} \times \cdots \times \Xi_{\overline{\pi}_i}^{\Pi(j_n)} (\Xi_{\overline{\pi}_i}^{\Pi(j_n)}) (\Xi_{\overline{\pi}_i}^{\Pi(j_1)})\tag{14}
\]
with $\Xi_j = [x_i + (j - 1)h_i, x_i + jh_i]$ and $h_i = \frac{x_i - x_i}{N}$. Then,
\[
X \setminus (\Xi \cup \Xi) \supseteq Y_{\text{int}} \cup Y_{\text{bnd}}.
\]
**Proof.** By construction, the function $f$ takes values larger than $\gamma$ on all interval boxes $\Xi_{\pi_i}^{\Pi(j_1)} \times \cdots \times \Xi_{\pi_i}^{\Pi(j_n)} (\Xi_{\pi_i}^{\Pi(j_n)})$ for any $j \in \mathcal{J}_k$. Similarly, $f$ takes smaller values than $\gamma$ on all intervals $\Xi_{\overline{\pi}_i}^{\Pi(j_1)} \times \cdots \times \Xi_{\overline{\pi}_i}^{\Pi(j_n)} (\Xi_{\overline{\pi}_i}^{\Pi(j_n)})$ for any $j \in \mathcal{J}_k$. Consequently, the union of all of these boxes cannot possibly contain a point of $Y_{\text{int}} \cup Y_{\text{bnd}}$, which is the statement of the theorem. \qed

Theorem 3 provides a constructive procedure for finding the desired outer approximation of the set $Y_{\text{int}} \cup Y_{\text{bnd}}$. Notice that the computational complexity of Algorithm 3 is of order $O(n_x N \log(N))$, because we need to sort the intervals along all coordinate directions. The associated storage complexity is of order $O(n_x N)$. Finally, we have
to keep in mind, however, that computing and storing the sets \( \Xi \) and \( \Xi^\prime \) is expensive in general, as these sets may be composed of an exponentially large amount of sub-intervals. Nevertheless, it is not necessary to store these sets explicitly as long as we store the permutation matrices \( \Pi \) and \( \Pi^\prime \) as well as the boxes \( J \) and \( J^\prime \), which uniquely represent the set \( X \setminus (\Xi \cup \Xi^\prime) \).

Notice that there are various heuristics possible for refining the above procedure. However, the corresponding methods are analogous to the implementation in SIVIA and based on state-of-the-art branching techniques. Thus, the proposed technique based on Algorithm 3 can be embedded in an exhaustive search procedure, if one wishes to approximate the set \( X_{\text{Int}} \cup X_{\text{bound}} \) with any given accuracy.

5. NUMERICAL EXAMPLES

This section illustrates some of the benefits of ISA as a bounding method for the range of factorable functions, as well as its application to GPE. Algorithms 1, 2, and 3 are implemented in the programming language Julia. For comparison, a basic SIVIA algorithm was also implemented in Julia. The termination for both algorithms was based on (7). All results were obtained on an Intel Xeon CPU X5660 with 2.80GHz and 16GB RAM.

5.1 Bounding a nonlinear function: ISMs vs TMs

Consider the nonlinear factorable function
\[
f(x) = \frac{\sin(z_1) + \sin(z_2)}{\cos(z_2)}
\]
over the domain \( X = [0, 1] \times [0, 2\pi] \). Here, \( \pi \in [0, 20] \) denotes a parameter which controls the diameter of the domain. In order to measure the quality of an arithmetic, we used the Hausdorff distance between the range of \( f \) and \( \overline{f} \), which does not increase monotonically with \( \pi \). Although the Hausdorff distance between \( f(X) \) and \( \overline{f} \) does not increase monotonically with \( \pi \), the rough trend observed on the plot is that the overestimation increases with the size of the domain. Furthermore, the plot shows that interval superposition models outperform Taylor models over large domains. One aspect that is not shown in the figure is that over small domains, e.g. over \([0, 10^{-1}]^2\), enclosures based on Taylor models outperform those constructed using interval superposition arithmetic.

5.2 Guaranteed parameter estimation via ISMs

We consider a reaction system given:
\[
\begin{align*}
\dot{z}_1(t) &= -(x_1 + x_3)z_1(t) + x_2z_2(t), & z_1(0) &= 1, \\
\dot{z}_2(t) &= x_1z_1(t) - x_2z_2(t), & z_2(0) &= 0, \\
\end{align*}
\]
with \( y(t) = z_2(2) \) (Paulen et al., 2016). The output variable, can be represented as the factorable function
\[
y(t) = \frac{e^{\frac{2t}{\sigma}}x_1(\frac{t}{\sigma} - e^{-\frac{t}{\sigma}})}{\sigma}
\]
with \( \sigma = \sqrt{x_1^2 + x_2^2 + x_3^2 + 2x_1p_1 + 2x_1x_2 - 2x_2x_3} \) as well as \( \rho = x_1 + x_2 + x_3 \). In the following, we fix \( x_3 = 0.35 \) and consider \( n_m = 15 \) measurements corresponding to the time instants \( t_i = 1, 2, \ldots, 15 \). Process measurements were obtained by simulating (16) with \( x = (0.6, 0.15, 0.35)^T \), rounding to the second significant digit. Measurement errors of \( \pm 10^{-3} \) were added to these values.

The performance of the proposed GPE algorithm using ISA was tested against a standard SIVIA. We have interval superposition models with \( N = 2 \), 10, 20. Figure 3 shows a summary of the results of the GPE algorithm using ISMs with \( N = 2 \). The left plot, shows an approximation of the set \( X_p \). The plot shows the inner partition (in red) for \( \epsilon = 10^{-5} \) and the boundary partitions for \( \epsilon = 10^{-4} \) (light blue) and \( \epsilon = 10^{-5} \) (dark blue). The central and right plots show, respectively, a comparison of the number of iterations and CPU time against the tolerance \( \epsilon \) for SIVIA (solid red line) and ISM-based set-inversion with \( N = 2 \) (solid black line), \( N = 10 \) (dotted black line), and \( N = 20 \) (dashed black line). In terms of the number of iterations and number of boundary boxes (not shown), ISM-based set-inversion (for all \( N \)) outperforms SIVIA. This is due to the fact that ISA is able to detect and exploit structures in the factorable function to remove redundant boxes. On the contrary, with respect to the CPU time, SIVIA outperforms the proposed algorithm. This can be traced back to the fact that the the cost per iteration is larger for ISA. Furthermore, the implementation is still at prototype stage and requires further refinement in terms of computing remainder bounds and memory management in the algorithms.

6. CONCLUSION

This paper presented Interval superposition arithmetics, a novel set-arithmetic for computing enclosures of the image set of factorable functions and its use in guaranteed parameter estimation. The main advantage of ISA is its polynomial storage and computational complexity. The core routine behind the proposed GPE method is the intersection of an interval superposition model and an interval. Although the proposed intersection routine has a computational complexity of order \( O(n_2N\log(N)) \), computing an arbitrarily accurate approximation of the
parameter set requires exponential run time. Our numerical examples illustrate the advantages of ISA over other set arithmetics when constructing enclosures for factorable functions—particularly over large domains. We have also shown how the proposed technique can be used to solve a GPE problem. Although the number of iterations is reduced when using ISA, the overall CPU time is larger than SIVIA. This suggest that, although ISA can improve certain aspects of GPE algorithms, there is still much room for improvement. Improved ISA-based algorithms for constructing approximations of inverse-image sets in polynomial run-time will be investigated in future work.

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