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Ellipsoidal Arithmetic for Multivariate Systems

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Abstract

The ability to determine enclosures for the image set of nonlinear functions is pivotal to many applications in engineering. This paper presents a method for the systematic construction of ellipsoidal extensions of factorable functions. It proceeds by lifting the ellipsoid to a higher dimensional space for every atom operation in the function DAG, thereby accounting for dependencies. We present theoretical results regarding the quadratic Hausdorff convergence of the computed enclosures. Moreover, we propose an efficient implementation, whereby the shape matrix of the lifted ellipsoid is stored in sparse format, and every atom operation corresponds to a sparse update in that matrix. We illustrate these developments with two numerical examples.

Keywords: Ellipsoids, Function Bounding, Interval Arithmetic

1. Introduction

The ability to compute tight enclosures of the image set of nonlinear functions is pivotal to many methods in global and robust optimization (Tawarmalani and Sahinidis, 2004; Stuber and Barton, 2011), reachability analysis (Althoff et al., 2008), uncertainty analysis (Rao and Berke, 1997), guaranteed parameter estimation (Jaulin and Walter, 1993), etc. For real-valued, factorable functions, interval arithmetic (Moore et al., 2009) provides a natural way of computing such enclosures, since the image set of any continuous function is itself an interval. In practice, an interval enclosure can be obtained by traversing a directed acyclic graph (DAG) of the function in order to bound its atom operations recursively and as tightly as possible (Schichl and Neumaier, 2005). Although simple, this approach suffers two main limitations, namely the dependency problem and the wrapping effect. The former happens when multiple occurrences of the same variable, e.g. in a complicated function expression, are treated as if they were independent from each other. The latter is due to the fact that the image of an interval vector under a vector-valued function, even a linear linear function, is generally not an interval vector itself, thus leading to overestimation in enclosing that image set with an interval vector (Lohner, 2001).

This paper presents a method for the systematic construction of ellipsoidal extensions of factorable functions. The algorithm starts with an ellipsoid containing the uncertainty host set and proceeds by adding an extra dimension (lifting) for every atom operation in the DAG. This is similar in essence to the construction of polyhedral relaxations using a decomposition-linearization approach (Tawarmalani and Sahinidis, 2004), with the added benefit of a well-developed ellipsoidal calculus (Kurzhanski and Vályi, 2004). We also analyze how fast the computed enclosures converge to the exact image as the uncertainty set is reduced, using the concept of Hausdorff convergence order (Bompadre and Mitsos, 2012), and we develop an efficient implementation as part of the software package MC++ (`https://projects.coin-or.org/MCpp`).

The remainder of the paper is organized as follows. After defining the problem in Sect. 2, we describe the construction of ellipsoidal extensions of factorable functions in Sect. 3. Theoretical results regarding the Hausdorff convergence of the computed enclosures are presented in Sect. 4. Then, we discuss important implementation details in Sect. 5, and illustrate mitigation of both the dependency and wrapping effects with numerical examples. Finally, Sect. 6 concludes the paper.

Notation. Besides standard mathematical notation, the diameter of a compact set $Z \subseteq \mathbb{R}^n$ is defined by $\mathrm{diam}(Z) = \max_{z1,z2\in Z} \|z_1 - z_2\|$. The Minkowski sum of two compact sets Z,W is $W \oplus Z := \{w+z \,|\, w \in W, z \in Z\}$. If $W \subseteq Z$ the Hausdorff metric between these sets is given by $d_{\mathrm{H}}(W,Z) := \max_{z\in Z} \min_{w\in W} \|w - z\|$. An n-dimensional ellipsoid is defined as:

$$\mathscr{E}(q,Q) \;:=\; \left\{ q + Q^{\frac{1}{2}} v \;\middle|\; \forall v \in \mathbb{R}^n,\; v^{\mathsf{T}} v \le 1 \right\} \;\in\; \mathbb{E}^n \;,$$

where $\mathbb{E}^n$ denotes the class of n-dimensional ellipsoids, the vector $q \in \mathbb{R}^n$ and the positive semidefinite matrix $Q \in \mathbb{S}_+^n$ are respectively the center and the shape matrix of the ellipsoid.

2. Problem Formulation

Consider a function $f : \mathbb{R}^{n_x} \to \mathbb{R}^{n_f}$, with its argument $x \in \mathbb{R}^{n_x}$ contained in the ellipsoid $\mathscr{E}(q_x,Q_x) \in \mathbb{E}^{n_x}$. The exact image of $\mathscr{E}(q_x,Q_x)$ under the function f is defined as

$$f\left(\mathscr{E}(q_x,Q_x)\right) \;:=\; \{ f(x) \,|\, x \in \mathscr{E}(q_x,Q_x) \} \,. \tag{1}$$

The main focus of this paper is on computing an enclosure of the image set of f in the form of an ellipsoid $\mathscr{E}(q_f,Q_f)$; that is, $\mathscr{E}(q_f,Q_f) \supseteq f\left(\mathscr{E}(q_x,Q_x)\right)$ with $(q_f,Q_f) \in \mathbb{R}^{n_f} \times \mathbb{S}_+^{n_f}$.

The main assumption we make to enable this construction is that the function f must be factorable, i.e. it can be decomposed into a finite number N of atom operations a_i from a finite library, such as binary addition, binary product, and outer composition with a univariate function. In particular, factorable functions can be evaluated by setting $u^0(x) = x$ and applying the recursive rule

$$\forall i \in \{1,\ldots,N\}, \quad u^i(x) \;=\; g_i(u^{i-1}(x)) \;:=\; \begin{pmatrix} u^{i-1}(x) \\ a_i(u^{i-1}(x)) \end{pmatrix} , \tag{2}$$

so that $f(x) = Pu^N(x) = P[g_N \circ g_{N-1} \circ \ldots \circ g_1](x)$, where $P \in \mathbb{R}^{n_f \times (n_x+N)}$ is a projection matrix selecting the appropriate components. The j-th component of $u^i(x)$ is denoted as $u^i_j(x)$ subsequently.

The main problem addressed in this paper is the development of a constructive approach for an ellipsoidal extension $f^{\mathbb{E}} : \mathbb{E}^{n_x} \to \mathbb{E}^{n_f}$ of the factorable function f, whose image $f^{\mathbb{E}}(q_x,Q_x)$ yields the ellipsoidal enclosure, $\mathbb{E}(q_f,Q_f) := f^{\mathbb{E}}(q_x,Q_x) \supseteq f(\mathscr{E}(q_x,Q_x))$.

3. Ellipsoidal Arithmetic for Factorable Functions

The proposed algorithm proceeds by lifting the ellipsoid to a higher dimensional space for every atom operation in the function's DAG upon application of an ellipsoidal arithmetic. Starting with an ellipsoid $\mathscr{E}(q^0,Q^0) \in \mathbb{E}^{n_x}$ with $q^0 := q_x$ and $Q0 := Q_x$, an ellipsoidal extension of each factor g_i, $i = 1,\ldots,N$ is obtained such that $g_i^{\mathbb{E}}(\mathscr{E}(q^{i-1},Q^{i-1})) = \mathscr{E}(q^i,Q^i)$, with

$$q^i := \begin{pmatrix} q^{i-1} \\ \lambda^i \end{pmatrix} \quad \text{and} \quad Q^i := \begin{pmatrix} I_{i-1} \\ \Lambda^i \end{pmatrix} Q^{i-1} \begin{pmatrix} I_{i-1} \\ \Lambda^i \end{pmatrix}^{\mathsf{T}} . \tag{3}$$

Here, $I_{i-1} \in \mathbb{R}^{(n_x+i-1)\times(n_x+i-1)}$ denotes the identity matrix; and the lifting parameters $\lambda^i \in \mathbb{R}$ and $\Lambda^i \in \mathbb{R}^{n_x+i-1}$ (row vector) depend on the functional form of the corresponding atom operation a_i.

At the end, the ellipsoidal extension $f^{\mathbb{E}}$ of f is retrieved by projecting the lifted ellipsoid $\mathscr{E}(q^N,Q^N) \in \mathbb{E}^{n_x+N}$ onto $\mathbb{R}^{n_f}$, giving

$$f^{\mathbb{E}}(q_x,Q_x) \;:=\; \mathscr{E}(q_f,Q_f) \;=\; P \times \mathscr{E}(q^N,Q^N) \,.$$

The following two subsections describe ways that such lifting parameters can be constructed for both linear and nonlinear atom operations.

3.1. Affine Atom Operations

Consider those operations $u^i(x) := g_i(u^{i-1}(x))$, where the atom operation a_i is an affine function of at most two factors $u_k^{i-1}(x), u_m^{i-1}(x)$ with $k,m \leq i-1$. This corresponds to the case of addition, subtraction, scaling and shifting.

Addition and Subtraction Operations, $u_k^{i-1}(x) \pm u_m^{i-1}(x)$. The lifting parameters are given by:

$$\lambda^i := q_k^{i-1} \pm q_m^{i-1} \quad \text{and} \quad \Lambda_j^i := \begin{cases} 1 & \text{if } j = k, \\ \pm 1 & \text{if } j = m, \\ 0 & \text{otherwise.} \end{cases} \tag{4}$$

Scaling Operation, $\alpha u_k^{i-1}(x)$ for some $\alpha \in \mathbb{R}$. The lifting parameters are given by:

$$\lambda^i := q_k^{i-1} \quad \text{and} \quad \Lambda_j^i := \begin{cases} \alpha & \text{if } j = k, \\ 0 & \text{otherwise.} \end{cases} \tag{5}$$

Shifting Operation, $u_k^{i-1}(x) + \beta$ for some $\beta \in \mathbb{R}$. The lifting parameters are given by:

$$\lambda^i := q_k^{i-1} + \beta \quad \text{and} \quad \Lambda_j^i := \begin{cases} 1 & \text{if } j = k, \\ 0 & \text{otherwise.} \end{cases} \tag{6}$$

3.2. Nonlinear Atom Operations

Consider the operation $u^i(x) = g_i(u^{i-1}(x))$, where the atom operation a_i is a possible nonlinear function of the sole factor $u_k^{i-1}(x)$ with $k \leq i-1$ first. Note that the domain $D_i \subseteq \mathbb{R}$ of a_i is given by the projection of the ellipsoid $\mathscr{E}(q^{i-1}, Q^{i-1})$ onto its k-th component, given by $D_i := q_k^{i-1} + \sqrt{Q_{k,k}^{i-1}}\,[-1,1]$. In particular, we make the assumptions that: (i) D_i is included within the domain of definition of a_i throughout—this is relevant, for instance, for the univariate functions $z \mapsto \log(z)$, $z \mapsto 1/z$, $z \mapsto \sqrt{z}$, etc; and (ii) the function a_i is Lipschitz continuous.

One way of handling the nonlinear factor g_i involves constructing a linear estimator such that

$$\forall v \in \mathscr{E}(q^{i-1}, Q^{i-1}), \quad g_i(v) := \begin{pmatrix} v \\ a_i(v) \end{pmatrix} \in \left\{ \begin{pmatrix} 0_{i-1} \\ \gamma_0^i \end{pmatrix} + \begin{pmatrix} I_{i-1} \\ \gamma_1^i e_k^\mathsf{T} \end{pmatrix} v \right\} \oplus \begin{pmatrix} \{0_{i-1}\} \\ [-\delta^i, \delta^i] \end{pmatrix}, \tag{7}$$

whereby the scalars γ_0^i, γ_1^i and δ^i can be derived, for instance, from a Taylor model or, better, a Chebyshev model of order $q \geq 1$ of the atom operation a_i on D_i (Neumaier, 2003; Rajyaguru et al., 2014); the latter is more advantageous in that it can be applied to nonsmooth atom operations, too. In (7), e_k stands for the kth basis vector and 0_{i-1} is a zero vector of size $i-1$.

The lifting operation proceeds in two steps. In the first step, the linear part of (7) is absorbed into the a lifted ellipsoid $\mathscr{E}(q^i, \tilde{Q}^i)$ in a procedure that is similar to the one used for shifting and scaling in (5)-(6), here with the lifting parameters

$$\lambda^i := \gamma_0^i \quad \text{and} \quad \Lambda_j^i := \begin{cases} \gamma_1^i / \operatorname{rad}(D_i) & \text{if } j = k, \\ 0 & \text{otherwise.} \end{cases} \tag{8}$$

In the second step the interval $[-\delta^i, \delta^i]$ which encloses the nonlinearity is added to the ith component of the lifted ellipsoid, in the Minkowski sense. Since the set of n-dimensional ellipsoids is not closed under Minkowski addition, we use an ellipsoidal extension of the Minkowski sum so that $\mathscr{E}(q^i, Q^i) := \mathscr{E}(q^i, \tilde{Q}^i) \oplus^{\mathbb{E}} \mathscr{E}(\Delta^i)$, with $\Delta^i := (\delta^i)^2(e_i e_i^\intercal) \in \mathbb{S}^{n_x+i}$. In particular, we compute the shape matrix Q^i as

$$Q^i := \frac{1}{\mu_0}\tilde{Q}^i + \frac{1}{\mu_1}\Delta^i \quad \text{with} \quad \mu_0 = 1 - \mu_1 = \frac{\sqrt{\mathrm{Tr}\left(\tilde{Q}^{i-1}\right) + \varepsilon}}{\sqrt{\mathrm{Tr}\left(\tilde{Q}^{i-1}\right) + \varepsilon} + \sqrt{\mathrm{Tr}\left(\Delta^i\right) + \varepsilon}} \,. \tag{9}$$

Finally, in the case of binary product operations, the atom operation a_i is a bilinear term between two factors $u_k^{i-1}(x)$, $u_m^{i-1}(x)$ with $k, m \le i-1$. Of the possible ways to yield an ellipsoidal enclosure of bilinear terms, we use a simple DC-decomposition approach here. After rewriting the bilinear term in the form

$$u_k^{i-1}(x) \times u_m^{i-1}(x) = \frac{1}{4}\left[(u_k^{i-1}(x) + u_m^{i-1}(x))^2 - (u_k^{i-1}(x) - u_m^{i-1}(x))^2\right] , \tag{10}$$

we can apply recursively the rules of binary addition/subtraction and univariate composition for the square function $z \mapsto z^2$, as explained earlier. As an alternative, and potentially tighter, approach, one can envisage the use of semi-definite programming (SDP) to handle bilinear terms.

4. Convergence Analysis

We now turn our attention to analyzing the theoretical convergence properties of the ellipsoidal arithmetic presented in the previous section. An ellipsoidal extension $f^{\mathbb{E}}$ of f is said to have Hausdorff convergence order $q \ge 1$ on $\mathbb{E}^{n_x}$ if

$$d_{\mathrm{H}}\left(f^{\mathbb{E}}(\mathscr{E}(q_x, Q_x)), f(\mathscr{E}(q_x, Q_x))\right) \;\le\; \mathbf{O}(\mathrm{diam}(\mathscr{E}(q_x, Q_x))^q) \,, \tag{11}$$

for every domain $\mathscr{E}(q_x, Q_x) \in \mathbb{E}^{n_x}$ with sufficiently small diameter where $f^{\mathbb{E}}$ is defined. The following result relates the convergence order of a factorable function to the convergence order of its atom operations.

Theorem 1. *If all the atom operations a_i in the DAG of a factorable function f are Lipschitz continuous and their ellipsoidal extensions have image Hausdorff convergence order q, then the ellipsoidal extension of f itself has image Hausdorff convergence q.*

Proof. The result follows by finite induction over the atom operations, using the triangle inequality for the Hausdorff metric d_{H} and the Lipschitz continuity of each atom operation a_i. □

We now present the main result of this section.

Theorem 2. *Let all the atom operations a_i in the DAG of a factorable function f be twice-continuously differentiable, and consider the ellipsoidal extension $f^{\mathbb{E}}$ of f as constructed from the lifting procedure in Sect. 3. Then, $f^{\mathbb{E}}$ has quadratic Hausdorff convergence on $\mathbb{E}^{n_x}$.*

Proof. We show that the ellipsoidal extension of each atom operation have quadratic Hausdorff convergence, so the result follows from Theorem 1 with $q = 2$. Since the class of ellipsoids is closed under affine transformations, all the extensions for affine atom operations in Sect. 3.1 are exact, and hence have infinite Hausdorff convergence order. Since binary product operations are handled by a combination of affine operations and univariate nonlinear operations, the Hausdorff convergence order of the extension $f^{\mathbb{E}}$ is completely determined by the Hausdorff convergence order of the latter. Consider the operation $g_i(u^{i-1}(x))$ where the atom operation a_i is a nonlinear function of the sole factor $u_k^{i-1}(x)$ with $k \le i-1$, and assume without loss of generality that $\mathscr{E}(q^{i-1}, Q^{i-1})$ is centered at zero (mainly for notation simplicity). By construction of $g_i^{\mathbb{E}}$ and invariance of ellipsoids under affine transformations, the ellipsoidal approximation $\mathscr{E}(\tilde{Q}^i)$ matches the exact image of the linear part in (7). The exact image of the corresponding residual term is

$$\Gamma := \left\{ g_i(v) - \begin{pmatrix} 0_{i-1} \\ \gamma_0^i \end{pmatrix} + \begin{pmatrix} I_{i-1} \\ \gamma_1^i e_k^\intercal \end{pmatrix} v \,\middle|\, v \in \mathbb{E}(Q^{i-1}) \right\} .$$

Then, we have:

$$\begin{aligned} d_{\mathrm{H}}\left(\mathscr{E}(Q^i), g_i(\mathscr{E}(Q^{i-1}))\right) &= d_{\mathrm{H}}\left(\mathscr{E}(\tilde{Q}^i) \oplus^{\mathbb{E}} \mathscr{E}(\Delta^i), \mathscr{E}(\tilde{Q}^i) \oplus \Gamma\right) \\ &\leq d_{\mathrm{H}}\left(\mathscr{E}(\tilde{Q}^i) \oplus^{\mathbb{E}} \mathscr{E}(\Delta^i), \mathscr{E}(\tilde{Q}^i)\right) + d_{\mathrm{H}}\left(\mathscr{E}(\tilde{Q}^i), \mathscr{E}(\tilde{Q}^i) \oplus \Gamma\right) \\ &\leq d_{\mathrm{H}}\left(\mathscr{E}(\tilde{Q}^i) \oplus^{\mathbb{E}} \mathscr{E}(\Delta^i), \mathscr{E}(\tilde{Q}^i)\right) + \mathbf{O}\left(\mathrm{diam}\left(\Gamma\right)\right) \\ &\leq \mathbf{O}\left(\mathrm{diam}\left(\mathscr{E}(\Delta^i)\right)\right) + \mathbf{O}\left(\mathrm{diam}\left(\Gamma\right)\right) , \end{aligned}$$

where the last inequality follows from the definition of the ellipsoidal extension of the Minkowski sum in (9). The result is obtained by noting that

$$\mathrm{diam}\left(\Gamma\right) \leq \mathbf{O}\left(\mathrm{diam}(\mathscr{E}(Q^{i-1}))^2\right) \quad \text{and} \quad \mathrm{diam}\left(\mathscr{E}(\Delta^i)\right) \leq \mathbf{O}\left(\mathrm{diam}(\mathscr{E}(Q^{i-1}))^2\right) ,$$

by the assumption that g_i is twice-continuously differentiable and by the Lipschitz-continuity of natural interval extensions, respectively. □

5. Numerical Implementation and Numerical Examples

Although simple, the algorithm describe in Sect. 3 is not the most effective way to implement the ellipsoidal arithmetic. Firstly, the number of atom operations N in the DAG of a factorable function is known a priori, which allows preallocation of the center vector and shape matrix. The second observation is that the lifting operation defined in (3) corresponds to an update in the ith row of the shape matrix; for instance, for an addition or subtraction operation $u_k^{i-1}(x) \pm u_m^{i-1}(x)$:

$$\forall j \in \{0, \ldots, i\}, \quad Q^i_{i,j} = \begin{cases} Q^i_{k,k} \pm 2Q^i_{k,m} + Q^i_{m,m} & \text{if } j = 1, \\ Q^i_{k,j} \pm Q^i_{m,j} & \text{otherwise.} \end{cases}$$

Therefore, an efficient implementation is possible, whereby the (symmetric) shape matrix of the lifted ellipsoid is stored in sparse format and every atom operation corresponds to a sparse update of the shape matrix. Such an implementation of the ellipsoidal arithmetic is available as part of the software package MC++ (`https://projects.coin-or.org/MCpp`).

We illustrate the benefits of ellipsoidal arithmetic compared with traditional interval arithmetic for two problems. The left plot in Fig. 1 considers the following factorable function with $n_x = n_f = 2$,

$$f_1(x_1, x_2) = \sqrt{x_1 + x_2} + x_1 x_2 \qquad f_2(x_1, x_2) = (x_1 - x_2)^2 + 3x_2 .$$

The comparison between the actual image set and the corresponding interval and ellipsoidal extensions, here for a variable host set $\mathscr{E}(q_x, Q_x)$ with $q_x = \begin{pmatrix} 3 \\ 4 \end{pmatrix}$ and $Q_x = \begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix}$, illustrates the potential of ellipsoidal arithmetic to mitigate the dependency problem.

The right plot of Fig. 1 shows the solution set of the parametric linear ODE (harmonic oscillator)

$$\dot{x}_1(t) = x_2(t) + p , \qquad \dot{x}_2(t) = -x_1(t) + p ,$$

with joint ellipsoidal host set $\mathscr{E}(q_{x,p}, Q_{x,p})$ for the initial states $x_1(0), x_2(0)$ and the parameter p given by $q_{x,p} = (1 \;\; 0 \;\; 0)^\intercal$ and $Q_{x,p} = 0.01 I_3$. The unconditional stability of the reach tube illustrates the ability of ellipsoidal arithmetic to mitigate the wrapping effect, which is due to the property of invariance under affine transformations of ellipsoids.

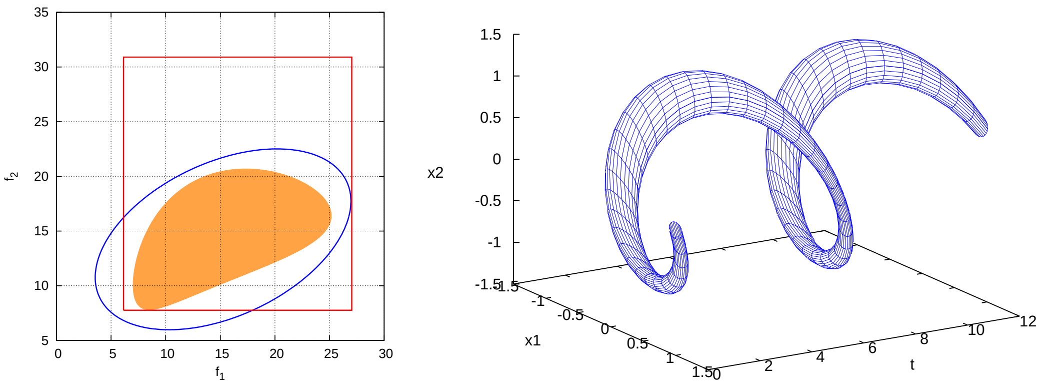

Figure 1: Left plot: Mitigation of the dependency problem using ellipsoidal arithmetic compared with interval arithmetic for a factorable function; Right plot: Mitigation of the wrapping effect by the property of invariance under affine transformation of ellipsoids for a parametric ODE.

6. Conclusion

This paper was concerned with the construction of ellipsoidal enclosures for the image set of factorable functions. Our approach provides such enclosures by traversing a DAG of the function, and it applies an ellipsoidal arithmetic that lifts the ellipsoid to a higher dimensional space for every atom operation. We have shown that this arithmetic yields quadratically convergent ellipsoidal extensions under mild assumptions, and that it can be implemented efficiently on account of sparsity. In practice, quadratic Hausdorff convergence is a very desirable property in branch-and-bound search for global optimization in order to reduce the cluster effect, as well as in the design of validated integrators for asymptotically stable systems. Further research is needed in order to extend existing interval-based algorithms to ellipsoidal techniques nonetheless.

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