Simulation Based Computation of Certificates for Safety of Dynamical Systems

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Abstract

In this paper, we present an algorithm for synthesizing certificates for safety of continuous time dynamical systems, so-called barrier certificates. Unlike the usual approach of using constraint solvers to compute the certificate from the system dynamics, we synthesize the certificate from system simulations. This makes the algorithm applicable even in cases where the dynamics is either not explicitly available, or too complicated to be analyzed by constraint solvers, for example, due to the presence of transcendental function symbols.

The algorithm itself allows the usage of heuristic techniques in which case it does not formally guarantee correctness of the result. However, in cases that do allow rigorous constraint solving, the computed barrier certificate can be rigorously verified, if desired. Hence, in such cases, our algorithm reduces the problem of finding a barrier certificate to the problem of formally verifying a given barrier certificate.

1 Introduction

A common technique in formal verification is the reduction of a verification problem to a constraint solving problem. A main limitation of such approaches comes from theoretical and practical limitations of the decision procedures used to solve the resulting constraints. In the case of continuous systems, this is usually the theory of the real numbers which is undecidable as soon as periodic function symbols, such as the sine function are allowed. Even in the polynomial case, which is decidable [37], existing decision procedures are by far not efficient enough to be able to solve realistic problems.
In contrast to that, simulations of continuous systems, approximating the solutions of the underlying differential equations, are possible for systems far beyond those restrictions.

In this paper, we circumvent the constraint solving bottleneck by using an approach that is data-driven instead of deductive: We use simulation data instead of system dynamics as the main input for computing certificates. From a given set of simulations we compute a candidate for a certificate. If this candidate turns out to not to be a certificate for the system itself, we use a refinement loop to run further simulations. In our concrete case, the certificates are formed by so-called barrier certificates [29].

The algorithm uses optimization as its main workhorse. Here, we allow sub-optimal results which enables the use of fast heuristic [22] and numerical [27] optimization algorithms. In cases, where the system dynamics can be handled by rigorous decision procedures, the final result can be rigorously verified. This final verification step is then applied to a barrier certificate that is already given. Hence it is a much easier problem than the computation of the barrier certificate itself. In our experiments, the non-verified results always turned out to be mathematically correct. Moreover, the final rigorous verification step always took negligible time. The experiments also show that the approach can compute barriers for ordinary differential equations of a complexity that has been out of reach for computation of barrier certificates up to now.

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2 Problem Description

Definition 1 A safety verification problem is a tuple \((\Omega, f, I, U)\) where

- \(\Omega \subseteq \mathbb{R}^n\) (the state space of the safety verification problem),
- \(f : \Omega \to \mathbb{R}^n\), Lipschitz continuous (the vector field or dynamics),
- \(I \subseteq \mathbb{R}^n\) (the set of initial states), and
- \(U \subseteq \mathbb{R}^n\) (the set of unsafe states).

We want to verify that a given safety verification problem does not have a solution of the ordinary differential equation \(\dot{x} = f(x)\) that leads from an
initial to an unsafe state. The corresponding decision problem is in general undecidable \[1\], and decidable only for very special cases \[14\]. Hence we head for an algorithm that successfully solves benchmark problems.

The following object \[29, 36\] certifies successful safety verification:

**Definition 2** A barrier certificate of a safety verification problem \((\Omega, f, I, U)\) is a differentiable function \(V\) such that

- \(\forall x \in I . V(x) < 0\),
- \(\forall x \in U . V(x) > 0\), and
- \(\forall x \in \Omega . V(x) = 0 \Rightarrow (\nabla V(x))^T f(x) < 0\).

In this paper, we will introduce an algorithm that, for an arbitrary given safety verification problem, tries to compute such a barrier certificate. If successful, this implies safety:

**Property 1** If a safety verification problem \((\Omega, f, I, U)\) has a barrier certificate, then there is no solution \(x : [0, T] \rightarrow \Omega\) of the ODE \(\dot{x} = f(x)\) such that \(x(0) \in I\) and \(x(T) \in U\).

Our approach is template based. That is, we introduce parameters into the function \(V\), resulting in a parametric function \(V(p, x)\) that we call template. This reduces the problem of finding a barrier to the problem of finding parameter values such that the template is a barrier. The template can have an arbitrary form, but we will usually work with polynomial templates, that is, templates of the form \(p_0 + \sum p_i \bar{x}^i\), where the \(\bar{x}_i\) are power products, and \(p_0, p_1, \ldots\) are parameters.

So, now we are left with the problem of finding a vector \(p\) of parameter values such that \(\forall x \in I . V(p, x) < 0\), \(\forall x \in U . V(p, x) > 0\), and \(\forall x \in \Omega . V(p, x) = 0 \Rightarrow (\nabla V(p, x))^T f(x) < 0\).

We denote the conjunction of these three constraints by \(C_f\). The constraint \(\exists p C_f\) represents a decision problem in the theory of real numbers with quantifier prefix \(\exists \forall\). In the polynomial case, this is decidable \[37\], function symbols such as \(\sin\) make the problem undecidable. However, even in the polynomial case, in practice, existing decision procedures can only solve problems with a few variables. Note also, that for a template with \(k\) parameters, this constraint has \(n + k\) variables.
3 Algorithmic Framework

Even if the dynamics $f$ is complex, it is usually possible to compute simulations of the system behavior. That is, for a given $x_0 \in \Omega$ and a time bound $T$, one can compute an approximation of the solution of the ordinary differential equation $\dot{x} = f(x)$ of length $T$, starting in $x_0$. Simulation is an essential tool in practical systems modeling, and approximation is usually taken into account already during the modeling process. As a consequence such simulations often describe the intended system behavior more accurately than even the precise mathematical solution.

We will represent such simulations by pairs $(s, s') \in \Omega \times \Omega$, where $s$ is the starting point, and $s'$ is the endpoint of the simulation. We will call such pairs simulation segments. The straightforward way of computing such a pair $(s, s')$ is to fix $s$ and a time bound $T$ and then to compute $s'$ using simulation. Note however, that it is also possible to do reverse simulation, that is to fix $s'$ and to compute $s$ by solving the ordinary differential equation $\dot{x} = -f(x)$.

We will maintain a set $S$ of such simulation segments. Our goal is to use this set $S$ for computing a solution $p$ of the constraint $C_f$. For this we relax the universal quantifiers to finite conjunctions. For the first two parts of the constraint $C_f$ we simply replace the set $I$ bounding the universal quantifiers in the first part with the set of all initial points in $S$, and the set $U$ with the set of all unsafe points in $S$. However, for the third part of $C_f$, due to the implication occurring here, it does not suffice to replace the set $\Omega$ by a finite subset. This would allow trivial satisfaction of this implication using a parameter vector $p$ such that $V(p, s) > 0$ for every element of this finite subset. Instead, we use the observation, that the third part of $C_f$—which ensures a certain direction of the vector field $f$ on the zero set of the barrier—implies that no solution of $\dot{x} = f(x)$ may connect a point with negative value of $V$ to a point with positive value of $V$. The resulting constraints are:

- $\bigwedge_{(s, s') \in S, I(s)} V(p, s) < 0$, $\bigwedge_{(s, s') \in S, I(s')} V(p, s') < 0$
- $\bigwedge_{(s, s') \in S, U(s)} V(p, s) > 0$, $\bigwedge_{(s, s') \in S, U(s')} V(p, s') > 0$
- $\bigwedge_{(s, s') \in S} V(p, s) > 0 \lor V(p, s') < 0$

We will call the conjunction of these constraints sampled constraint and will denote it by $C_S$. Clearly, this approximation of $C_f$ by $C_S$ does not lose barrier certificates:
Property 2 $C_f$ implies $C_S$.

Unlike the original constraint $C_f$, the sampled constraint $C_S$ does not contain any quantifier alternation which makes it easier to solve. However, it may have spurious solutions, that is, solutions that do not correspond to a solution of the original constraint and that, hence, do not represent a barrier certificate.

In order to handle such a situation, we use the following property:

Property 3 If $S \subseteq S'$ then $C_{S'}$ implies $C_S$.

So adding more segments to $S$ does not weaken the approximation. To actually strengthen the approximation we use an algorithm based on the principle of counter-example based refinement: The algorithm computes a solution of $C_S$ that we will call barrier candidate, checks whether this barrier candidate is spurious, and if yes, generates and adds a counter-example in the form of a new simulation segment that refutes the given barrier candidate. If the barrier candidate is not spurious, we return the vector $p$ which then represents a barrier certificate.

The resulting algorithm looks as follows:

initialize $S$ with some simulation segments
let $p$ be s.t. $p \models C_S$
while $p \not\models C_f$ do
  $S \leftarrow S \cup \{(s, s')\}$, where $(s, s')$ is a simulation segment with $p \not\models C_{S \cup \{(s, s')\}}$
  let $p$ be s.t. $p \models C_S$
return $p$

The algorithm leaves the concrete choice of the barrier candidate and counter-example open. As it is, allowing an arbitrary choice of those objects, it does not work. The main problem is a consequence of the fact that the space of barrier candidates is uncountable. Computing an arbitrary barrier candidate, and then removing this single barrier candidate does, in general, not make enough progress in removing spurious barrier candidates.

Moreover, if the system dynamics $f$ is non-polynomial, it is, in general, not possible to decide the satisfiability test $p \models C_f$ which is the termination condition of the algorithm.

In the next three sections we will design a variant of the above algorithm that overcomes those problems. We will compute a barrier candidate $p$ s.t.

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1Decision procedures for real closed fields, can circumvent this problem [15], due to the fact that semi-algebraic sets possess an algorithmically computable finite cellular decomposition [4].
\( p \models C_S \) and a counter-example \((s, s')\) with \( p \not\models C_{S \cup \{(s, s')\}} \) that ensure as much progress of the algorithm as possible. As a side-effect we will also get a termination condition for the refinement loop that represents a computable and practically reliable replacement for the satisfiability test \( p \models C_f \).

4 Computing a Barrier Candidate

The sampled constraint \( C_S \) can have many solutions. Which one should we choose? Certainly we should prefer non-spurious solutions that is, solutions that also satisfy the original constraint \( C_f \). Moreover, if a solution turns out to be spurious, removing it should remove as many further spurious solutions as possible. We will work with the assumption, that those objectives will be fulfilled by solutions that are as central as possible in the solution set of the sampled constraint.

For this we replace the inequalities, that can be either satisfied or not, by a finer measure [30]. Observing, that the right-hand side of every inequality is zero, we base this measure on the value of the term on the left-hand side: This value measures how strongly a given point \( p \) satisfies a greater-than-zero predicate. In the case of a less-than-zero predicate, we can measure this by multiplying the value of the term on the left-hand side by \(-1\). Moreover, we replace conjunction by the minimum operator and disjunction by the maximum operator in the style of fuzzy logic.

The result is the function

\[
\min \left\{ \begin{array}{l}
\min_{s \in I, (s, s') \in S} -V(p, s), \\
\min_{s' \in I, (s, s') \in S} -V(p, s'), \\
\min_{s \in U, (s, s') \in S} V(p, s), \\
\min_{s' \in U, (s, s') \in S} V(p, s'), \\
\min_{(s, s') \in S} \max\{V(p, s), -V(p, s')\}
\end{array} \right. 
\]

which we maximize to find points that satisfy the constraint \( C_S \) as strongly as possible.

Now observe that template polynomials \( V(p, x) \) of the form \( p_0 + \sum p_i x^i \) are linear in their parameters \( p_0, p_1, \ldots \). Hence, the result of substituting points \( s \) and \( s' \) for \( x \) in \( V(p, x) \) is a linear inequality of the form \( a^T p < 0 \) with \( p \) being the parameter vector \((p_0, p_1, \ldots)\) and \( a \) being a vector of real numbers whose first entry, resulting from the monomial \( p_0 \), is the constant 1.

For a polynomial template and \( \lambda \geq 0 \), \( V(\lambda p, s) = \lambda V(p, s) \). Hence, also the above function scales in such a way, the corresponding optimization problem is unbounded, and optimization algorithms will usually simply come up with larger and larger values for the vector \( p \). In other words, instead of optimizing for our goal of being as much as possible in the solution set
of the sampled constraint this formulation optimizes for large parameter values which, in turn, result in large values of \( V(p, s) \). We avoid this by constraining the (max)-norm of the vector \( p \) to not to exceed 1.

However, even then, minimizing a linear term \( a^T p \) enforces large distance from the boundary of the solution set of \( C_S \), if \( ||a|| \) is small, and vice versa. For avoiding this, we normalize the terms, resulting in \( \frac{a^T}{||a||_2} p \). This amounts to computation of the Chebyshev center \(^2\), that is, the center of the largest ball contained in the solution set.

So we solve the optimization problem

\[
\max_{\|p\| \leq 1} F_S(p)
\]

where \( F_S(p) \) is the minimax function above with all linear terms normalized by dividing them with the 2-norm of their coefficients.

**Property 4** \( F_S(p) > 0 \) iff \( p \models C_S \)

Hence, a positive result of the optimization problem gives us a solution of the sampled constraint. By optimizing further, we get solutions that are as central as possible in the solution set of \( C_S \), hence also increasing the chances of finding a solution of the original constraint \( C_f \).

## 5 Computing a Counter-Example

The solution \( p \) of the sampled constraint \( C_S \) might be spurious, that is, it might not satisfy the original constraint \( C_f \). If the computed solution is spurious, we generate a counter-example, that is, a new simulation segment \((s, s')\) s.t. \( p \) does not satisfy the strengthened sampled constraint \( C_{S \cup \{(s, s')\}} \). However, this constraint should not only refute the computed barrier candidate \( p \), but as many further spurious solutions as possible. The techniques from the previous section, that is, maximizing \( F_S \) instead of computing an arbitrary solution of \( C_S \), alleviates the problem. However, in addition, we also want to add a simulation segment \((s, s')\) that removes as many spurious solutions as possible.

For this we again translate the constraint solving problem of finding a counter-example into an optimization problem. However, searching for a strong violation of \( C_{S \cup \{(s, s')\}} \) by searching for a simulation segment \((s, s')\)

\(^2\)Note that due to the disjunction, we do not have a polyhedron here. Still, this formulation models the Chebyshev center.
s.t. $F_{S\cup \{(s,s')\}}$ is minimal, is an ODE-constrained optimization problem. Such problems are notoriously difficult to solve. In order to avoid this, we work with the original constraint $C_f$, instead.

We have a fixed barrier candidate $p$ and look for an $x$ violating one of the individual parts of $C_f$. By looking for an $x$ violating one of the individual parts of $C_f$ as much as possible we hope to construct a counter-example not only for the given spurious candidate $p$, but for as many further spurious candidates as possible.

Applying the constraint-to-function transformation already described in the previous section to the three parts of the constraint $C_f$, we arrive at the functions

\[
\min \{-V(p, x) \mid x \in I\}, \quad \min \{V(p, x) \mid x \in U\}, \quad \min \{-\nabla V(p, x)^T f(x) \mid V(p, x) = 0, x \in \Omega\}.
\]

However, the third entry does not fully correspond to the original intention of the corresponding constraint: Its task is to measure, whether all solution of the ODE crossing the zero level set $\{x \mid V(p, x) = 0\}$ do so in the correct direction. This direction should be independent wrt. scaling of $f(x)$ or $\nabla V(x)$. In order to normalize those factors, we replace the objective function $-\nabla V(p, x)^T f(x)$ with the objective function

\[
\frac{-\nabla V(p, x)^T f(x)}{||\nabla V(p, x)|| \cdot ||f(x)||}.
\]

As a result, we have three optimization problems,

- $\min_{x \in I} F_I(p, x)$, where $F_I(p, x) := -V(p, x)$,
- $\min_{x \in U} F_U(p, x)$, where $F_U(p, x) := V(p, x)$, and
- $\min_{x \in \Omega, V(p, x) = 0} F_{\nabla V}(p, x)$ where $F_{\nabla V}(p, x) := -\frac{-\nabla V(p, x)^T f(x)}{||\nabla V(p, x)|| \cdot ||f(x)||}$.

Compared to the problem from the previous section, where the search space is the parameter space, and the state space was discretized, here $p$ is fixed, and we search in the original state space $\Omega$.

Denoting the endpoint of a solution of length $T$ of the ODE $\dot{x} = f(x)$ starting in $x_0$ by $\phi(x_0, T)$, we have:

**Property 5** Let $x \in I$ with $F_I(p, x) < 0$. Then for all $T \geq 0$, $p \not\models C_{S\cup \{(x,\phi(x,T))\}}$.

**Property 6** Let $x \in U$ with $F_U(p, x) < 0$. Then for all $T \geq 0$, $p \not\models C_{S\cup \{(\phi(x,-T),x)\}}$. 


Property 7 Let \( x \) be such that \( V(p, x) = 0 \) and \( F_{\nabla}(p, x) < 0 \). Then there is a \( T^* > 0 \) s.t. for all \( 0 < T \leq T^* \), \( p \nmid C_{S \cup \{ (\phi(x,-T), \phi(x,T)) \}} \).

So we add simulation segments approximating \((x, \phi(x,T)), (\phi(x,-T), x)\), and \((\phi(x,-T), \phi(x,T))\), respectively. In the case of \((\phi(x,-T), \phi(x,T))\) we have to be careful to not to do too long simulations, due to the upper bound \( T^* \) in Property 7.

6 Resulting Algorithm

initialize \( S \) with some simulation segments

\[(cand, cntrxpl) \leftarrow \text{check}(S)\]

\textbf{while} \( \neg [\text{cand} = \bot \lor \text{cntrxpl} = \emptyset] \) \textbf{do}

\[S \leftarrow S \cup \text{cntrxpl}\]

\[(cand, cntrxpl) \leftarrow \text{check}(S)\]

\textbf{if} \( \text{cand} = \bot \) \textbf{then return} “no barrier found”

rigorously verify \( \text{cand} \)

\textbf{return} \( \text{cand} \)

\textbf{optional verification step}

subalgorithm \text{check}(S): returns barrier candidate and counter-example

let \( p \) be s.t. \( F_{S}(p) \) is as large as possible

\textbf{compute a barrier candidate}

\textbf{if} \( F_{S}(p) \leq 0 \) \textbf{then return} \((\bot, \emptyset)\)

no barrier candidate found

let \( x_I \in I \) be s.t. \( F_I(p, x_I) \) is as small as possible

let \( x_U \in U \) be s.t. \( F_U(p, x_U) \) is as small as possible

let \( x_{\nabla} \in \Omega \) be s.t. \( V(p, x_{\nabla}) = 0 \) and \( F_{\nabla}(p, x_{\nabla}) \) is as small as possible

\[m \leftarrow \min\{F_I(p, x_I), F_U(p, x_U), F_{\nabla}(p, x_{\nabla})\}\]

\textbf{if} \( m \geq 0 \) \textbf{then return} \((p, \emptyset)\)

no counterexample found

\textbf{return} \((p, \{(s, s')\})\) where

\[(s, s') = \begin{cases} 
\text{a forward simulation from } x_I, \text{if } m = F_I(p, x_I) \\
\text{a backward simulation from } x_U, \text{if } m = F_U(p, x_U) \\
\text{a forward/backward simulation from } x_{\nabla}, \text{if } m = F_{\nabla}(p, x_{\nabla}) 
\end{cases}\]

Note that here we only need values for which the objective functions are large (small, respectively). We do not insist on a lower bound of the minimization problem (upper bound on the maximization problem, respectively), let alone a decision procedure. This allows the use of various heuristic optimization techniques [22] that even can be applied in cases where finding a precise optimum is impossible due to non-decidability issues, for example, due to non-polynomial system dynamics \( f \) occurring in \( F_{\nabla} \).
Also observe that the optimization of $F_S(p)$ is a search problem of the parameter space dimension $k$, and the computation of $x_I$, $x_U$, and $x_\nabla$ is a search problem of the state space dimension $n$. In contrast to that, directly solving original constraint $C_f$ is a problem in dimension $n + k$.

The final step of rigorously verifying the barrier candidate, that is, verifying $p \models C_f$, is a problem in state space dimension $n$, as well. Due to the strategy of optimizing for a barrier candidate, the computed candidate will usually satisfy $C_f$ robustly. Hence, even in undecidable cases, this allows the application of procedures that exploit robustness [31].

7 Implementation

In the section, we show how the optimization problems and the final verification step of the algorithm from the previous section can be solved in practice.

As described in Section 4, $F_S(p)$ is linear in $p$. However, it contains a min/max alternation which is beyond the capabilities of usual numerical optimization algorithm. The key to solving this constraint is the observation that the min/max operators occurring within $F_S(p)$ are finite. Hence the optimization problem can be rewritten to the following constrained optimization problem: Maximize $\delta$ under

$$\bigwedge_{(s,s') \in S,I(s)} -V(p,s) \geq \delta, \bigwedge_{(s,s') \in S,I(s')} -V(p,s') \geq \delta,$$

$$\bigwedge_{(s,s') \in S,U(s)} V(p,s) \geq \delta, \bigwedge_{(s,s') \in S,U(s')} V(p,s') \geq \delta,$$

$$\bigwedge_{(s,s') \in S} V(p,s) \geq \delta \lor -V(p,s') \geq \delta.$$

This is an optimization modulo theory [26, 33] problem in the theory LRA (linear real arithmetic).

For minimizing $F_I(p,x)$, $F_U(p,x)$, and $F_\nabla(p,x)$ one can use classical numerical optimization [27]. Since such methods do local search, they may run into local, but non-global optima. To search for global solutions one can start several optimization runs from random starting points which is also known under the term multi-start [23]. Note that this is trivial to parallelize efficiently.

For the final rigorous verification step, one can use a simple branch-and-bound approach, evaluating the terms $V(p,x)$ using interval arithmetic [25], checking the inequalities of Definition 2 on the resulting intervals, and using splitting to tighten the bounds, if necessary.
8 Computational Experiments

We did experiments with a prototype implementation of the method described so far. The prototype requires the state space, set of initial states and the set of unsafe states to have the shape of a hyper-rectangle. We initialize the set \( S \) by forward simulations from all vertices of the initial hyper-rectangle and backward simulations from all vertices of the unsafe hyper-rectangle. Due to this initialization, our prototype implementation does not check barrier candidates for violations of the first two conditions of Definition 2 and indeed, even without such a check, the computed barriers do not violate those conditions.

For each example, we set the lengths of all simulations manually to a certain constant \( \sigma \) that we show below. Moreover, we cancel simulations that leave a bloated version of the state space. Here, we simply bloat each interval bound of \( \Omega \) by a certain percentage from its distance from the interval center:

\[
bloat([a, b]) = \left[ a + \frac{b}{2} - b(a + \frac{b}{2} - a), a + \frac{b}{2} + b(a - \frac{b}{2}) \right] = \left[ \frac{(1+b)a+(1-b)\pi}{2}, \frac{(1-b)a+(1+b)\pi}{2} \right].
\]

In our experiments, we use \( b = 1.1 \).

The examples that we used are:

1. a standard ODE modeling a pendulum with normalized parameters (e.g., Kapinski et al. [18], Example 1), where the variable \( x \) models the angle of the pendulum, and \( y \) models angular speed.

\[
\begin{align*}
\dot{x} &= y \\
\dot{y} &= -\sin x - y
\end{align*}
\]

\( \Omega = [-10, 10] \times [-10, 10], \ I = [-10, 10] \times [8, 10], \ U = [-10, 10] \times [-10, -5], \sigma = 0.5 \)

2. dynamics from [5, Example 5]

\[
\begin{align*}
\dot{x} &= y + (1 - x^2 - y^2)x + \ln(x^2 + 1) \\
\dot{y} &= -x + (1 - x^2 - y^2)y + \ln(y^2 + 1)
\end{align*}
\]

\( \Omega = [-5, 5] \times [-5, 5], \ I = [1, 3] \times [-1.5, 3.0], \ U = [-3, -0.6] \times [1, 3], \sigma = 1 \)

3. a standard Lorenz system [38], see also [6, Example 7]

\[
\begin{align*}
\dot{x} &= 10(y - x) \\
\dot{y} &= x(28 - z) - y \\
\dot{z} &= xy - \frac{8}{3}z
\end{align*}
\]
\[ \Omega = [-20, 20] \times [-20, 0] \times [-20, 20], \quad I = [-14.8, -14.2] \times [-14.8, -14.2] \times [12.2, 12.8], \quad U = [-16.8, -16.2] \times [-14.8, -14.2] \times [2.2, 2.8], \quad \sigma = 0.1 \]

4. composition of trivial dynamics (variable \( x_1 \)) and pendulum (variables \( x_2 \) and \( x_3 \))

\[
\begin{align*}
\dot{x}_1 &= 1 \\
\dot{x}_2 &= x_3 \\
\dot{x}_3 &= -10 \sin x_2 - x_3
\end{align*}
\]

\[ \Omega = [-10, 10]^3, \quad I = [9, 10] \times [-10, 10]^2, \quad U = [-10, -9] \times [-10, 10]^2, \quad \sigma = 0.1 \]

5. scalable example, manually constructed

\[
\begin{align*}
\dot{x}_1 &= 1 + \frac{1}{t} \left( \sum_{i \in \{1, \ldots, l\}} x_{i+1} + x_{i+2} \right) \\
\dot{x}_2 &= x_3 \\
\dot{x}_3 &= -10 \sin x_2 - x_2 \\
\vdots \\
\dot{x}_{2l} &= x_{2l+1} \\
\dot{x}_{2l+1} &= -10 \sin x_{2l} - x_2
\end{align*}
\]

\[ \Omega = [-10, 10]^{2l+1}, \quad I = [9, 10] \times [-10, 10]^{2l}, \quad U = [-10, -9] \times [-10, 10]^{2l}, \quad \sigma = 0.1, \text{ with } l = 1 \]

6. same as Example 5 but \( l = 2 \)

7. same as Example 5 but \( l = 3 \)

8. same as Example 5 but \( l = 4 \)

All experiments were executed on a notebook with Intel(R) Core(TM) i7-5600U CPU @ 2.60GHz and running Ubuntu Linux 16.10. For simulation we used the software package CVODE version 2.5.0 from the SUNDIALS suite of solvers. For optimizing \( F_S(p) \) we use the tool OptiMathSAT [34]. For minimizing \( F_I(p, x), F_U(p, x), \) and \( F_V(p, x) \) we use the function sqp from the software package GNU Octave 4.0.3 which implements the optimization method of sequential quadratic programming. We globalized this method by multi-start with 16 local optimization runs. For the final rigorous verification step, we use our software RSolver (http://rsolver.sourceforge.net) which extends a basic interval branch-and-bound method with interval constraint propagation.

We list the results in Table 1. Here, the column “dim” denotes the problem dimension and “templ” denotes one of the following templates:
Table 1: Results of Experiments

| dim | templ | iter | simulation | candidate | counter-example | verif |
|-----|-------|------|------------|-----------|----------------|-------|
| 1   | 2     | Q    | 10         | 0.24      | 1.2            | 8.21  | 0    |
| 2   | 2     | Q    | 5          | 0.11      | 0.25           | 5.7   | 0.41 |
| 3   | 3     | T    | 10         | 0.3       | 1.01           | 17.03 | 0    |
| 4   | 3     | L    | 1          | 0.02      | 0              | 1.07  | 0    |
| 5   | 3     | L    | 1          | 0.01      | 0.01           | 1.21  | 0    |
| 6   | 5     | L    | 1          | 0.14      | 0.36           | 3.51  | 0    |
| 7   | 7     | L    | 1          | 1.06      | 7.38           | 7.67  | 0    |
| 8   | 9     | L    | 1          | 15.81     | 1340.6         | 19.76 | 0.01 |

**Q:** \( p_0 + p_1 x^2 + p_2 xy + p_3 y^2 + p_4 x + p_5 y \)

**T:** \( p_0 + p_1 x^2 + p_2 x + p_3 y \)

**L:** the linear template \( p_0 + p_1 x_1 + \cdots + p_n x_n \) with \( n \) being the state space dimension

Moreover, the column “iter” denotes the number of iterations of the refinement loop. Further columns denote the time spent in simulation, computation of a barrier candidate, computation of a counter-example, and verification. The time unit are seconds.

As can be seen, in all cases, the computed barrier could be rigorously verified. Moreover, the time needed to do so is negligible. The whole method scales to higher-dimensional examples, but as the problem dimension increases, the optimization module theory solver used to compute a barrier candidate is increasingly becoming a bottleneck. Note that we used the solver as a black box, with the original parameter settings.

To ensure verifiability of our results, we list the computed barriers:

1. \( 0.118462553528y^2 - 0.011722981249xy - 0.709542580128y - 0.0550927673883x^2 - 0.0586149062452x - 1 \)
2. \( 0.408692986165y^2 - 0.386033509251xy - 0.227005969996y + 0.0866893912879x^2 - 0.925807829028x - 1 \)
3. \( (-z) + 0.086216517173x^2 + 0.406513973333x - 0.668459116412 \)
4. \( 0.12774317671 - x_1 \)
5. \( 6.94919072662 \times 10^{-4} x_3 + 7.29701934574 \times 10^{-4} x_2 - x_1 + 0.127740909365 \)
6. \( 0.00298446742425x_5 - 0.00705872836204x_4 - 0.00693382587388x_3 + 0.00295825595803x_2 - x_1 + 0.100721787174 \)
9 Related Work

The original method for computing barrier certificates [29] was based on sums-of-squares programming [28]. Since then, various further methods for computing barrier certificates and inductive invariants of polynomials systems have been designed [32, 12, 19, 40, 39, 10].

To the best of our knowledge, there is only one method capable of computing barrier certificates for non-polynomial systems [6]. The method is not based on simulation but uses interval-based constraint solving techniques, in a similar way as we do in the final verification step, and in a similar way as the algorithm implemented in RSolver [31]. This restricts the method to systems where such techniques are available, which corresponds to those systems, where our algorithm can do the final verification step. The method applies branching to both the state and parameter space, whereas our algorithm, at a given time, always searches only in one of the two. Instead of our method for computing barrier candidates, the method guesses barrier certificates by simply trying midpoints of intervals which can be very efficient if this guess happens to be lucky, but very inefficient, if not. Especially, if the midpoint of the user-provided parameter space already happens to be a barrier certificate, then the method succeeds without any search. Unfortunately, the paper does not give any information on the computed barriers, which makes comparison difficult.

The approach to generalize or learn system behavior from simulations has been used before for computing Lyapunov functions [18, 17] and for computing the region of attraction [20]. Simulations can also be used to directly verify system behavior [11, 8, 7, 9]. For an overview of simulation-based approaches to systems verification see Kapinski et al. [16].

In software verification, the usage of test runs was shown to be useful in the computation of inductive invariants [13, 35]. However, the problem and solution are quite different from what we have here due to the discrete nature of both time and data types occurring in computer programs.

Our algorithm can also be interpreted as an online machine learning [24] process that learns a barrier certificate from simulations, querying for new
simulations to improve the barrier certificate. Moreover, the samples reachable from an initial state or leading to an unsafe state can be interpreted as positive and negative examples. However, here we do not have a classification problem due to the third property of Definition 2.

10 Conclusion

In this paper, we have presented an approach for synthesizing barrier certificates from system simulations. The resulting method is able to compute barrier certificates for ODEs that have been out of reach for such methods so far.

In the future we will increase the usability of the method by automatizing the choice of the used template and by automatically adapting the length of the computed simulation. We will also combine the method with falsification methods [21] that search for ODE solutions that lead from an initial to an unsafe state. In such a combined method, falsification should exploit the result of failed attempts at computing a barrier certificate and vice versa.

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