Constrained Optimization for Falsification and Conjunctive Synthesis

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Abstract. The synthesis problem of a cyber-physical system (CPS) is to find an input signal under which the system’s behavior satisfies a given specification. Our setting is that the specification is a formula of signal temporal logic, and furthermore, that the specification is a conjunction of different and often conflicting requirements. Conjunctive specifications are often challenging for optimization-based falsification—an established method for CPS analysis that can also be used for synthesis—since the usual framework (especially how its robust semantics handles Boolean connectives) is not suited for finding delicate trade-offs between different requirements. Our proposed method consists of the combination of optimization-based falsification and constrained optimization. Specifically, we show that the state-of-the-art multiple constraint ranking method can be combined with falsification powered by CMA-ES optimization; its performance advantage is demonstrated in experiments.

1 Introduction

Optimization-Based Falsification Falsification is a major approach to quality assurance of cyber-physical systems. The problem is formulated as follows.

Problem 1.1 (Falsification Problem).

– **Given:** a model $\mathcal{M}$ that takes an input signal $u$ and yields an output signal $\mathcal{M}(u)$, and a specification $\varphi$

– **Find:** a falsifying input, that is, an input signal $u$ such that the corresponding output $\mathcal{M}(u)$ violates $\varphi$

Optimization-based falsification is an established approach to finding a falsifying input, initiated in [5]. The key concept of optimization-based falsification is translation of Problem 1.1 into minimization of “how robustly” $\mathcal{M}(u)$ satisfies the specification $\varphi$. As we will see in §2 such a degree is incarnated by the robust semantics, which assigns a real number $[\mathcal{M}(u), \varphi] \in \mathbb{R} \cup \{-\infty, -\infty\}$ to an output signal $\mathcal{M}(u)$ and a specification $\varphi$. This allows us to utilize existing optimization algorithms to adaptively choose prospective input signals $u$ and eventually find
a falsifying input. Furthermore, one easily figures out that falsification of \( \neg \varphi \), namely the problem to find a falsifying input for \( \neg \varphi \), is equivalent to synthesis of \( \varphi \), namely the problem to find an input that satisfies \( \varphi \).

**Conjunctive Synthesis** The goal of the paper is to exploit and extend the techniques for optimization-based falsification for the purpose of solving the following conjunctive synthesis problem.

**Problem 1.2** (Conjunctive Synthesis).

- **Given:** a model \( M \) that takes an input signal \( u \) and yields an output signal \( M(u) \), and a conjunctive specification \( \varphi \equiv \varphi_1 \land \cdots \land \varphi_m \)
- **Find:** a satisfying input, that is, an input signal \( u \) such that the corresponding output \( M(u) \) satisfies \( \varphi \)

Instances of conjunctive synthesis are omnipotent in the real-world system design processes.

**Example 1.3.** Here is our leading example. The system model \( M \) is given by the Simulink model for automatic transmission from [4]—a system model commonly used in the falsification literature. The model \( M \) has two input (throttle, brake) and three output (rpm, speed, gear). The specification \( \varphi \) is given by

\[
\text{AT\_BRK-IN}_p := \Diamond_{[0,30]}(\text{rpm} \leq p) \land \Diamond_{[0,30]}(\text{speed} \leq 60) \land \Diamond_{[0,30]}(\text{gear} \geq 3) ;
\]

(1)

it means the gear should reach the third without any of RPM and speed getting too large, a requirement common in the break-in procedure. The RPM bound \( p \) is a parameter: the smaller \( p \) is, the harder the synthesis problem becomes.

Conjunctive synthesis is often hard. For example, the above leading example has conflicting requirements in the specification \( \varphi \)—gear gets larger typically when RPM and/or speed are larger, while the specification asks for RPM and speed to stay small—and satisfying all these requirements asks for a careful trade-off between them. Automated synthesis of input signals that achieve such delicate trade-offs (between performance and energy-efficiency, safety and progress, etc.) can help system designers who would otherwise spend a lot of time for manual trials and search.

**The Scale Problem** It is obvious that Problem 1.2 is equivalent to falsification of \( \neg \varphi \), suggesting the use of a falsification solver as an approach. However, existing falsification solvers can struggle with some problem instances, as we will see in §4. The main obstacle is the scale problem, a general problem in falsification that is identified and tackled in [9].

To illustrate the scale problem, consider our leading example where the specification AT\_BRK-IN\_p is given in (1). As we will see in the next section,
the robust semantics $[[M(u), \text{AT}_\text{BRK-IN}_p]] \in \mathbb{R} \cup \{\infty, -\infty\}$ of the formula $\text{AT}_\text{BRK-IN}_p$ is given by

$$[[M(u), \text{AT}_\text{BRK-IN}_p]] = v_1 \cap v_2 \cap v_3,$$

where

$$v_1 = \bigcap_{t \in [0,30]} (p - \text{rpm}(t)), \quad v_2 = \bigcap_{t \in [0,30]} (60 - \text{speed}(t)), \quad v_3 = \bigcup_{t \in [0,30]} (\text{gear}(t) - 3).$$

(2)

This expression clearly shows that, to make $[[M(u), \text{AT}_\text{BRK-IN}_p]] > 0$, all the three values $v_1, v_2, v_3$ should be positive simultaneously.

The issue here is that the formulation (2) can prevent hill-climbing optimization algorithms from effectively making all the three values $v_1, v_2, v_3$ positive. For example, imagine that we are in an early stage of the search for a satisfying input signal, and that all the values $v_1, v_2, v_3$ are still negative. By the nature of the automatic transmission model $M$, the value $v_1$ is likely to be in the order of (minus) thousands, the value $v_2$ is likely to be in the order of (minus) tens, and the value $v_3$ is either $-2$ or $-1$. In this case, the value $v_1$ dominates the overall objective function $v_1 \cap v_2 \cap v_3$, masking the contribution of $v_2$ and $v_3$. This obviously does not help finding a delicate balance between $v_1, v_2$ and $v_3$.

This problem—that some specific component dominates the robustness of a Boolean combination and masks away the other components—is exhibited in [9] where it is called the scale problem. A solution is proposed in [9] where conjuncts or disjuncts are thought of as arms in the multi-armed bandit problem (MAB) and an MAB algorithm is combined with an hill-climbing optimization solver. However, this solution in [9] is dedicated to satisfying the specifications of the form $\diamond (\varphi_1 \lor \varphi_2)$ and $\diamond (\varphi_1 \land \varphi_2)$, and therefore it does not apply to our current problem of conjunctive synthesis (satisfying $\varphi_1 \land \varphi_2 \land \cdots \land \varphi_m$, Problem 1.2).

Conjunctive Synthesis by Constrained Optimization

Our proposed method for solving conjunctive synthesis combines optimization-based falsification and constrained optimization—optimization of the value of a single objective function but subject to potentially multiple constraints. Specifically, we show that the state-of-the-art multiple constraint ranking method (MCR) [7] can be combined with CMA-ES [6], an optimization algorithm that is commonly used for the purpose of falsification. Our experimental results indicate clear performance advantage over an existing falsification solver (we compare with Breach [2]).

2 Conjunctive Synthesis by Constrained Optimization

Our specifications $\varphi \equiv \varphi_1 \land \cdots \land \varphi_m$ are given by STL formulas, as is common in the falsification literature. Their Boolean semantics $u \models \varphi$ is defined in a usual manner—it is much like for LTL formulas but takes additional care of the continuous notion of time.

The robust semantics $[[u, \varphi]]$ of an STL formula $\varphi$ under a signal $u$ is the key enabler of optimization-based falsification [5,8]. It takes an (extended) real
number as its value (\([u, \varphi] \in \mathbb{R} \cup \{\infty, -\infty\}\)), and satisfies the following key properties:

\[ [u, \varphi] > 0 \iff u \models \varphi, \quad [u, \varphi] < 0 \iff u \not\models \varphi. \quad (3) \]

Also noting that the robust semantics interprets conjunction \(\land\) by the infimum \(\sqcap\) of real numbers, Problem 1.2 is reformulated as follows. Consider the following optimization problem:

\[
\max_u [M(u), \varphi_1 \land \cdots \land \varphi_m], 
\text{ that is, }
\max_u [M(u), \varphi_1] \sqcap \cdots \sqcap [M(u), \varphi_m].
\quad (4)
\]

Once \(u\) is found such that the above robustness value is positive, this \(u\) is a solution to conjunctive synthesis (Problem 1.2), by (3). This is (the de Morgan dual of) the very idea behind optimization-based falsification.

However, the form (4) that uses infimum \(\sqcap\) often hinders hill-climbing optimization—this is the scale problem that we discussed in §1. The main idea of the paper is to regard conjuncts not as objectives (as in (4)) but as constraints, as below.

**Problem 2.1 (Conjunctive Synthesis by Multiple-Constraint Optimization).** In the setting of Problem 1.2 consider the following constrained optimization problem:

\[
\max_u [M(u), \varphi_1] 
\text{ subject to } [M(u), \varphi_i] > 0, \quad i = 2, \ldots, m.
\quad (5)
\]

Once \(u\) is found such that the robustness \([M(u), \varphi_1]\) is positive, this \(u\) is a solution to conjunctive synthesis (Problem 1.2), by (3). In (3), we picked \(\varphi_1\) as the optimization target, leaving the other conjuncts \(\varphi_2, \ldots, \varphi_n\) as constraints. We can do so without loss of generality since the order of the objectives is irrelevant. In practice, we would pick as \(\varphi_1\) the formula that we expect to be the most challenging to falsify.

Via the translation of Problem 1.2 to Problem 2.1 we make the major challenge in Problem 1.2 explicit in the problem formulation: the conflict between different conjuncts \(\varphi_1, \ldots, \varphi_m\) is buried away in a single objective function in (4); it is made explicit in (5). However, this translation would lead to an efficient solution only if there exists an algorithm that successfully exploits the structure that is now made explicit. This is the topic of the next section.

**Remark 2.2.** We note that Problem 2.1 is a single-objective optimization problem under multiple constraints, that should be distinguished from a multi-objective optimization problem. The latter’s notion of optimality is more involved (given e.g. by the Pareto front), and it would call for very different algorithms. Recall that our ultimate goal is constraint satisfaction \([M(u), \varphi_1] > 0, \ldots, [M(u), \varphi_m] > 0\). We need the robustness value of each formula \(\varphi_i\) to be positive, but we do not need to further maximize these values.
3 Our Algorithm: Combining MCR and CMA-ES

3.1 CMA-ES and the Constrained Optimization Taxonomy

Our baseline is the covariance matrix adaptation evolution strategy (CMA-ES) [6], an evolutionary optimization algorithm whose efficiency in the context of optimization-based falsification is well-established [9]. Here is its outline.

**Definition 3.1 (CMA-ES [6]).** Given a fitness function $f$, CMA-ES operates in an iterative manner, repeating the following regenerational steps until termination. Let $\mu, \lambda$ be fixed natural numbers with $\mu < \lambda$.

1. Generate a population $X = \langle u_1, u_2, \ldots, u_\lambda \rangle$ by sampling from the distribution $d_\theta$ on the search space, with the parameter value $\theta$ that is previously chosen. Specifically, the distribution $d_\theta$ is a Gaussian distribution, and $\theta$ gives its mean and covariance matrix.
2. Select $\mu$ individuals $u_{1:}\lambda, u_{2:}\lambda, \ldots, u_{\mu:}\lambda \in X$ that are the fittest on $f$.
3. Update the distribution parameter $\theta$ according to the selected individuals. Specifically, the new mean is the mean of the selected individuals $u_{1:}\lambda, \ldots, u_{\mu:}\lambda$, and the new covariance matrix is chosen in a suitable manner. See [6].

In search of a disciplined method for handling multiple (possibly conflicting) constraints, we turned to the taxonomy of constrained optimization problems [1]. According to the taxonomy, our current problem (Problem 2.1) is classified as follows.

- **Simulation-based** as opposed to **a priori**, in the sense that the satisfaction of a constraint is determined only in a black-box manner (we assume a model $\mathcal{M}$ is complex and thus black-box).
- **Relaxable** as opposed to **unrelaxable**, in the sense that the objective function has well-defined values even if the constraints are not satisfied.
- **Quantifiable** as opposed to **nonquantifiable**, in the sense that the degree of satisfaction of each constraint can be quantified (namely by the robustness $[\mathcal{M}(u), \varphi_i]$).

We note that constraint handling in CMA-ES is previously pursued in [8]. Their focus is however on a priori constraints, instead of simulation-based constraints that is our current setting.

3.2 MCR in CMA-ES

It turns out that the multiple constrained ranking algorithm (MCR) [7] fits the very classification discussed in the above. It works with general evolutionary optimization algorithms, hence also with CMA-ES.
Definition 3.2 (MCR in CMA-ES). Assume the setting of Problem 2.1 and let us write \( f(u) = [M(u), \varphi_1] \) for the optimization objective (the fitness function).

MCR in CMA-ES consists of replacing the use of the fitness function \( f \), in Step 2 of Def. 3.1 with the following scoring function \( F_X \). It also relies on the current population \( X \).

For each individual \( u \), the value \( F_X(u) \) is a natural number, and those \( u \) with smaller \( F_X(u) \) are deemed fitter. Its value is defined by

\[
F_X(u) = \begin{cases} 
\text{RVNum}_X(u) + \sum_{j=2}^{m} \text{RCon}_X^j(u) & \text{if no "feasible solution" in population } X, \\
\text{RObj}_X(u) + \text{RVNum}_X(u) + \sum_{j=2}^{m} \text{RCon}_X^j(u) & \text{otherwise.}
\end{cases}
\]

(6)

Here a “feasible solution” is an individual \( u \) that satisfies all the constraints, that is, \( [M(u), \varphi_i] > 0 \) for all \( i = 2, \ldots, m \). The functions \( \text{RVNum}_X, \text{RObj}_X, \text{RCon}_X^j \) all returns a suitable “rank” of the input. Specifically,

- \( \text{RObj}_X(u) \) is the rank of \( u \) among the population \( X \) in the descending order of the value of \( f \). That is, \( \text{RObj}_X(u_1) = 1 \) if \( f(u_1) \) is the greatest among \( \{ f(u) \mid u \in X \} \).
- For each \( j \in [2, m] \), \( \text{RCon}_X^j(u) \) is the rank of \( u \) among the population \( X \) in the descending order of the value of 0 ∩ \( [M(\_), \varphi_j] \), that is, the opposite of the degree of violation of constraint \( \varphi_j \). This is much like \( \text{RObj}_X(u) \) but note that the degree of satisfaction (i.e. positive robustness) is disregarded.
- \( \text{RVNum}_X(u) \) is the rank of \( u \) among \( X \) in the ascending order of the number of violated constraints, that is, for how many \( j \) we have \([M(u), \varphi_j] \leq 0 \).

Example 3.3. In the setting of Example 1.3. let \( \varphi_1 \equiv \Box(rpm \leq p) \), \( \varphi_2 \equiv \Box(speed \leq 60) \), \( \varphi_3 \equiv \Diamond(gear \geq 3) \) and assume that we have a population \( X = [u_1, u_2, u_3] \) where the robustness \([M(u_i), \varphi_j] \) \((i, j = 1, 2, 3)\) is obtained as described in Table 1.

In this case, the usual semantics indicates the input \( u_1 \) is the best individual among \( X \), in the sense that the infimum is the closest to 0. However, the input \( u_1 \) is in fact one in which \text{brake} is the maximum and \text{throttle} is 0 all the time. This is far from the satisfying input signal that we are after, but it is deemed to be the best among \( u_1, u_2, u_3 \) because the scale of the robustness of \( \varphi_3 \) is small (the scale problem).

On the other hand, the scoring function from MCR gives different values, as described in Table 2. We note that the formula \( \varphi_1 \equiv \Box(rpm \leq p) \) is picked as the objective (in Problem 2.1 and Definition 3.2) and the others \( \varphi_2, \varphi_3 \) as constraints. The scoring function \( F_X \) indicates the best input is \( u_2 \), which keeps the gear low and modestly violates \( u_1 \). In light of our requirement which asks for a careful trade-off between \( \varphi_1, \varphi_2, \varphi_3 \), it is natural to expect \( u_2 \) is more promising than \( u_1 \).

4 Experiments

Our implementation is based on Breach. In place of the MATLAB implementation of CMA-ES used in Breach, we plugged in \textit{pycma} (a standard Python
Table 1. Example; robustness of $\varphi_1, \varphi_2, \varphi_3$ for each individuals and their infimum

| Individual | $\varphi_1$ | $\varphi_2$ | $\varphi_3$ | infimum |
|------------|-------------|-------------|-------------|---------|
| $u_1$      | 1400        | 59.9        | -2          | -2      |
| $u_2$      | -9          | 2           | 1           | -9      |
| $u_3$      | -180        | 2           | -1          | -180    |

Table 2. Example; values of ranks and scoring function for each individuals

| Individual | $RObj_X$ | $RCon_1^X$ | $RCon_2^X$ | $RVNum_X$ | $F_X$ |
|------------|----------|-------------|-------------|------------|-------|
| $u_1$      | 1        | 1           | 3           | 2          | 7     |
| $u_2$      | 2        | 1           | 1           | 1          | 5     |
| $u_3$      | 3        | 1           | 2           | 2          | 8     |

implementation of CMA-ES [6] that is further combined with MCR (also implemented in Python). The latter communicates with Breach via the Python interface of MATLAB.

Our experiments used the system model $M$ and the specification $\varphi$ in Example 1.3, where we used the conjunct $\Box(rpm \leq p)$ as the objective ($\varphi_1$ in Problem 2.1) and the other two conjuncts $\Box(speed \leq 60), \Diamond(gear \geq 3)$ as constraints. The experiments were executed on a MacBook Pro 13-inch from 2018, 2.3 GHz Quad-Core Intel Core i5, 16 GB RAM.

We compared the performance of our algorithm (“MCR”) with that of the following:

- (“Breach”) Breach 1.7.0 (https://github.com/decyphir/breach) with its original MATLAB implementation of CMA-ES as the optimization solver; and
- (“Breach_pycma”) Breach 1.7.0 with the pycma implementation of CMA-ES as the optimization solver (without combination with MCR).

In Table 3, it is clear that the combination with MCR is advantageous in solving our target problem (the conjunctive synthesis problem, Problem 1.2), especially for its harder instances. More extensive experiments with other specs and system models are future work.

Table 3. Experimental results. SR shows success rates (out of 10 trials); time is the average execution time for successful trials in seconds.

| Spec, $\varphi$ | Breach | Breach_pycma | MCR (ours) |
|-----------------|--------|--------------|------------|
|                 | SR time | SR | time | SR | time |
| AT_BRK-IN_{2500} | 7 39.4 | 10 | 75.1 | 10 | 118.3 |
| AT_BRK-IN_{2400} | 1 70.0 | 2 | 209.0 | 9 | 255.9 |
| AT_BRK-IN_{2300} | 0 0 0 | 8 | 51.6 |
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