Bayesian Optimisation with Formal Guarantees

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Abstract—Application domains of Bayesian optimization include optimizing black-box functions or very complex functions. The functions we are interested in describe complex real-world systems applied in industrial settings. Even though they do have explicit representations, standard optimization techniques fail to provide validated solutions and correctness guarantees for them. In this paper we present a combination of Bayesian optimisation and SMT-based constraint solving to achieve safe and stable solutions with optimality guarantees.

I. INTRODUCTION

Bayesian optimization (BO) [1], [2] is a popular technique for optimizing an objective function \( f \), which is done through searching for input points \( x \) such that \( f(x) \) approximates the maximum \( \max f \). We refer to these points \( x \) as near-optimal. BO does not require an explicit representation of \( f \), and instead search for near-optimal points is based on sampling the values of \( f \) at a limited number of input points. BO is therefore used mainly for optimizing functions whose evaluation is expensive. In particular, BO is often used for hyper-parameter optimization when training machine learning models [3]. During the last few decades, BO has been used extensively for designing engineering systems [4].

BO iteratively builds a statistical model of \( f(x) \) usually from a prior distribution defined by a Gaussian process [5]. At each iteration \( i \) the current model is used to select the most promising candidate point \( x_i \) to evaluate the objective function \( f(x_i) \). This evaluation is used to update the posterior belief of the model. This process is repeated until some bound on the number of iterations is reached.

BO behaves well in practice and usually can find near-optimal points in just a few iterations. Nevertheless BO has its limitations. In particular, since BO is based on statistical approximations, there are no formal guarantees that the result achieved after a finite number of iterations is actually optimal or even close to optimal. Another limitation of BO is that even if the found point is near optimal the solution may not be stable: there may be close points on which the value of the objective function is very different from the optimum. Such solutions are undesirable in many applications which require regions around solutions to be also near optimal. This motivates combination BO with SMT-based constraint solving to achieve both safe and stable solutions which we develop in this paper.

In this work we are interested in applying optimization techniques to optimize microprocessor design, in particular, analog components that can be modelled as real-valued functions. In this context, the assumption that the objective function is very expensive to sample is no longer valid. Instead, achieving tighter approximations to the maximum \( \max f \) becomes more important even if computing near-optimal points that further improve the approximation accuracy becomes significantly more expensive. Besides, in this context, it is important to guarantee that the computed near-optimal point \( x \) satisfies the design constraints and it is robust [6] in the sense that small perturbations to \( x \) still yield legal near-optimal points for the objective function \( f \).

We propose a BO algorithm with the following properties:

- **Safety:** The computed near-optimal points are feasible (satisfy design constraints). In BO the feasibility of computed near-optimal solution is achieved by sampling the constraints [7]. In contrast, in our approach we use the explicit representation of the constraints to guide the search for a feasible near-optimal point.

- **Stability:** The computed near-optimal points are stable in the sense that perturbations within user-specified regions preserve output within near-optimal value. Stability is a critical requirement from analog devices because the inputs and the output can be perturbed due to uncertainties in the environment such as uncertain operating conditions, design parameter tolerances or actuator imprecisions [8]. This concept is studied in the BO setting as robustness [8], [9], [10], where it can be estimated with high confidence but cannot be proven formally.

- **Accuracy:** Our algorithm can find safe and stable near-optimal points for which the value of the objective function \( f \) is within a predefined distance from the real maximum, \( \max f \). This is enabled by the fact that in our problem setting the objective function and the constraints are given explicitly: probabilistic methods cannot provide full guarantees due to a limited number of sampling of \( f \).

The paper is organized as follows. In the next section we introduce the notation. In Section III we recall the basics of BO and in Section IV we define the stability and accuracy requirements from near-optimal solutions. In Section V we recall the algorithm for computing safe and stable configurations from [11] and present a BO algorithm that combines the strengths of reasoning with probabilities (Bayesian inference) and constraint solving (SMT). Experimental results are presented in Section VI. We conclude in Section VII.
II. PRELIMINARIES

Given a function \( f : A \rightarrow B \), by \( \text{dom} f \) we denote its domain \( A \). Vectors \((x_1, \ldots, x_n)\) may occur in the abbreviated form \( \mathbf{x} \). Given \( a, b \in \mathbb{R}^n \) with \( a_i \leq b_i \) for all \( i \), by \([a, b]\) we denote the Cartesian product \( \prod_{i=1}^{n} [a_i, b_i] \) of their component-wise closed intervals \([a_i, b_i]\). In this paper we consider formulas over \( (\mathbb{R}, 0, 1, \mathcal{F}, P) \), where \( P \) are the usual order predicates \( <, \leq, \text{etc.} \) and \( \mathcal{F} \) contains addition, multiplication with rational constants and some non-linear functions for example ReLU : \( x \mapsto \max\{0, x\} \), that can be used to encode complex objective functions represented by neural networks. Throughout, \( x, y \) denote variables in formulas while \( a, b, c, d, e, S, T \) stand for rational constants; both forms may be indexed. Whenever we use a norm \( \| \cdot \| \), we refer to the Chebyshev norm \( \| \mathbf{x} \|_\infty \). This basic BO algorithm does not take as input guarantees that the computed near-optimal points are feasible, with an SMT procedure where needed, as a building block of the solution is. We use this basic BO algorithm, complemented further from the real maximum the computed near-optimal solution is. We use this basic BO algorithm, complemented on a BO solver \( \text{A}^{\max}_{\text{BO}} \) for maximising \( f(x) \).

Algorithm 1 Basic optimisation algorithm using the BO solver \( \text{A}^{\max}_{\text{BO}} \) for maximising \( f(x) \).

\[
\text{MaxIter} - \text{a bound on the number of sampling iterations}
\]

Sample \( f \) at \( n_0 \) input points based on a heuristic:

Let \( x_i \in [a, b] \) and \( y_i = f(x_i) \) for \( i = 1, \ldots, n_0 \)

\( A \leftarrow \text{A}^{\max}_{\text{INIT}}(a, b, (x_i, y_i)_i) \)

\( \text{for } n = n_0 + 1, \ldots, \text{MaxIter} \) do

\( x_n \leftarrow \text{A}.\text{SUGGEST} \)

\( \text{Sample } y_n = f(x_n) \)

\( A \leftarrow \text{A}.\text{OBSERVE}(x_n, y_n) \)

end

\( y_j \leftarrow \max\{y_1, \ldots, y_{\text{MaxIter}}\} \)

return a near-optimal solution: \((x_j, y_j)\)

stable, with values close to the real maximum up to arbitrary given accuracy. We will define stability and accuracy formally in the next section.

IV. STABILITY AND ACCURACY

Given a real-valued function \( f \) on a bounded set \( X \subset \mathbb{R}^n \), we are interested in finding a maximum \( f(x^*) \) which is stable, in particular, for all values \( x' \) within a specified region around \( x^* \), \( f(x') \) stays within a specified threshold \( \varepsilon \) from \( f(x^*) \). This region around \( x^* \) is formalized as a stability guard \( \theta(x^*, x') \) which we assume is a reflexive binary relation over \( \text{dom } f \). This region could for example be defined by fixed radius or one relative to \( ||x|| \), but could also take a more complicated shape and we do not impose any restrictions on it besides that of being encodable as a quantifier-free formula \( \theta \). We assume \( f \) is encoded as the formula \( F(x_1, \ldots, x_n, y) \) over variables \( x_1, \ldots, x_n \) corresponding to the \( n \) inputs and \( y \) corresponding to the output \( f(x_1, \ldots, x_n) \).

Given a stability guard \( \theta \) for \( f \) and a bounded subset \( X \) of \( \text{dom } f \), we are addressing the optimisation problem

\[
\max_{x} \min_{x'} f(x') \quad \theta(x^*, x')
\]

on \( X \), and how to find reliable lower and upper bounds on the optimum \( y^* \), as well as a corresponding \( x^* \). That is, given a precision \( \varepsilon > 0 \), we want to compute \( T \) and a point \( x \in X \) such that \( T \leq y^* < T + \varepsilon \) and \( T \leq f(x') \) holds for all \( x' \) in the stability region around \( x \). In particular, \( T \) is an approximation of \( y^* \) accurate up to \( \varepsilon \). In the next section, we present algorithms based on combination of BO and SMT that solve this problem.

V. OPTIMISATION PROCEDURE

The problem (1) is equivalent to:

\[
\max \ y \text{ s.t. } \exists x (\forall x' \forall y' (\theta(x, x') \land F(x', y') \rightarrow y \leq y')).
\]

The type of formulas restricting \( y \) in (2) are also known to be in the \textsc{Gear}-fragment [11] of \( \exists \forall^* \) formulas.

We first recall the decision procedure \textsc{GearSat} [11] shown in Algorithm [2] which we enhance with BO solvers below. It takes a potential bound \( T \) and either verifies \( T \) to be
a lower bound on the optimum \( y^* \) or proves it to be an upper bound on \( y^* \). \textsc{GearsAT}_\( \delta \) alternates two phases: search for candidate solution and search for counter-example for stability around the candidate solution. It does that by first finding a point \( x \) for which \( f(x) \geq T \) holds – a candidate for a stable, accurate solution. If there is none, clearly \( T \) is an upper bound on \( y^* \). Otherwise, it checks whether \( x \) is seen as the center of the stability region \( \theta(x, \cdot) \), there is a counter-example \( x' \), that is, \( \theta(x, x') \) holds but \( f(x') \geq T \) does not (represented by \( D_i(x', y') \) constraint in Algorithm 2).

In the case when there are no counter-examples with that property, we can be sure that \( \theta(x, x') \implies f(x') \geq T \) for all \( x' \in X \). Otherwise, \( x' \) is a counter-example and the algorithm excludes the region \( \theta(\cdot, x') \) around it from the search for the next candidate. The stability condition \( \theta \) guides the proof search by generating lemmas excluding regions around counter-examples.

Here, \( \delta \geq 0 \) refers to a constant which can be used to ensure that solutions have a distance of at least \( \delta \) from regions defined by \( \theta \) containing counter-examples to safety of \( F \). This is done by learning lemmas of the form \( -\theta\delta(x, d) \) for each counter-example \( d \), where \( \theta\delta \) is the \( \delta \)-relaxation of \( \theta \) defined by

\[
\exists z \left( \|x - z\| \leq \delta \wedge \theta(x, d) \right).
\]

Termination of \textsc{GearsAT}_\( \delta \) was shown in [11]. We can use \textsc{GearsAT}_\( \delta \) to find an optimal value with a precision \( \epsilon \) on the value by a binary search of lower and upper bounds on the optimal value of the objective function: \( T \leq y^* < T + \epsilon \).

The key search parts in \textsc{GearsAT}_\( \delta \) rely on finding points (either candidates or counter-examples). One way to achieve this is by using an SMT solver to find points satisfying corresponding constraints (as done in [11]) but this can be computationally expensive. In this work we propose to delegate the search part to BO and the certification part to SMT checks. In this way we take the best from both worlds: efficient search in complex spaces from BO and formal guarantees on the optimisation results from SMT.

Our algorithms do not depend on particular types of BO and SMT solvers used. We only assume that the SMT solver supports quantifier-free fragment including formulas \( F \) and \( \theta \). Let us note that SMT solvers can handle a range of non-linear functions including polynomials, transcendental functions such as combinations of sine, cosine, exponentials and solutions of differential equations [12], [13], [14], [15].

First we integrate BO into \textsc{GearsAT}_\( \delta \) for searching counter-examples. We note that whenever \( \theta\delta(c_i, x') \) is equivalent to membership in the Cartesian product \( [a_i, b_i] \) (as is always the case in our application), Bayesian optimisation lends itself well to implement the search for a counter-example by solving \( D_i(x', y) \), as is shown in Algorithm 3. This works by starting a new minimising BO search in \( [a_i, b_i] \) once Algorithm 2 found a candidate \( c_i \).

Next, we integrate BO for finding candidate solutions. For this we need to guide BO to generate points outside of regions excluded by generated lemmas. Even though most BO solvers do not support constraints like the lemmas \( -\theta\delta(x, d_m) \) learnt by Algorithm 2 when \( X \subseteq \text{dom } f \) is equivalent to membership in \( [a_i, b_i] \) for some \( a_i, b_i \), it is still possible to use them in the search for a candidate \( e \) in our setting.

We achieve this by penalising any suggestion \( e \) that satisfies \( \theta\delta(x, d_{m_i}) \), for any counter-example \( d_{m_i} \), with the minimal value of a counter-example found when generating the lemma. This is shown in Algorithm 4. Alongside the SMT solver it maintains the maximising BO solver \( A_i \) that is initialised by \( A_i \leftarrow A_{\text{max INIT}}(a_i, b_i, e_j, f(e_j))_j \) for selected points \( e_j \in X \) which are either generated in previous iterations or randomly.

Note that due to penalising any of \( A_i \)’s suggestions inside regions containing counter-examples the function \( A_i \) observes is not necessarily \( f \). Whenever \( A_i \)’s suggestion \( c \) lies in a region around a previous counter-example \( d_{m_i} \) for some \( m < i \), that is, \( \theta(c, d_{m_i}) \) holds, we make \( A_i \) believe that the value of the function it optimises is \( f(d_{m_i}) \) instead of \( f(c) \). Since \( d_{m_i} \) was a counter-example to safety of \( F \), specifically \( f(d_{m_i}) < T \), this has the effect of penalising the suggestion \( c \) since it has already been proved to be \( \theta \)-close to a counter-example. We call \textsc{GearsAT}_\( \delta \) with integrated BO for counter-examples and candidate search \textsc{GearsAT}_\( \delta \)-BO. As shown next, this exchange of candidates and counter-examples between BO and SMT solvers proved to be beneficial in our experiments.
Algorithm 4 Finding candidates: Solving $C_i(x, y)$ with Bayesian optimisation and SMT in the $i$-th iteration of Algorithm 2 $A_i$ maximises.

if $i > 1$ then record previous counter-example $A_i \leftarrow A_{i-1}.\text{OBSERVE}(c_{i-1}, f(d_{i-1}))$

for $j = 1, \ldots, \text{MaxIter}$ do BO
  $c_i \leftarrow A_i.\text{SUGGEST}$
  if $\theta(c_i, d_m)$ for any $m \in \{1, \ldots, i-1\}$ then
    $z \leftarrow f(d_m)$ $\triangleright c_i$ is excluded by lemmas
  else
    $z \leftarrow f(c_i)$ $\triangleright c_i$ is an eligible candidate
  if $z \geq T$ then return $c_i$ $\triangleright f(c_i) \geq T$
  $A_i \leftarrow A_i.\text{OBSERVE}(c_i, z)$ $\triangleright z < T$
end
$c_i \leftarrow \text{solution of } C_i(x, y) \text{ restricted to } x \text{ or unsat } \triangleright \text{SMT}$

VI. BENCHMARKS

GEARSAT$_\delta$-BO is implemented in our solver called SMLP. As Bayesian optimizers $A^{\text{max}}, B^{\text{min}}$, we used the ones in the skopt library [16] based on Gaussian processes, with acquisition function $\text{gp\_hedge}$. The SMT part is implemented using the state of the art solver Z3 [12].

We evaluated GEARSAT$_\delta$-BO (presented in Section V) on 6 industrial examples from the Electrical Validation Lab at Intel. These are neural network models representing signal integrity of transmitters and receivers of a channel to a peripheral device. This application requires solutions to be safe and stable (see, Section IV), moreover the radii of stability regions are required to be proportional to the value of their respective centres. We evaluated all 4 combinations with and without BO-guided searches for candidates and counter-examples, respectively. These results are shown in Table II. In the left-most column $i$ refers to the problem instance, $c$ to whether BO search was used for candidates and $d$ to whether BO search was used for counter-examples. Observations:

- Throughout our experiments, the combination of BO with SMT solvers proved to find the best bound $T = 1$ to the optimum, whereas SMT alone timeouts in many cases.
- This can be attributed to the facts that a) when BO failed to find counter-examples ($n_{\text{ax}}$), none did exist ($N_{\text{ax}}$), and that b) the average time taken to find a counter-example is much shorter for BO ($t_{\text{ce}}/n_{\text{ce}}$) than for SMT ($T_{\text{ce}}/N_{\text{ce}}$ for $N_{\text{ce}} \neq 0$ results). This suggests that BO constitutes a very good heuristic for finding counter-examples.
- In addition, it turns out that as long as the total number of candidates found by BO-solver $A$ remains low ($n_{\text{cap}} < 50$), the asymptotically cubic complexity of the Gaussian process appears to be negligible compared to the overhead of rigorously solving the existential candidate formula by SMT. On the other hand, this advantage vanishes quickly after that, which motivates employing a kind of restart process similar to that successfully practised by current SAT and SMT solvers – at least for the BO solver $A$. Initial experiments suggest that training samples for the restarted BO solver require careful selection.
- The combinations *:0:1 correspond to those where BO tries to refute stability of SMT candidates. Throughout, it manages to do that with on average $n_{\text{ce}}/n_{\text{ce}} < 3$ tries (iterations) in Algorithm 3. On the other hand, for *:1:1 when BO tries to find counter-examples to BO candidates, this average with value $\approx 8.8$ is much higher on average in our experiments. This suggests that the quality of BO candidates when guided by BO counter-examples (case *:1:1) compares favourably to that of the SMT candidates with BO counter-examples (case *:0:1).
- All in all, we can see BO and SMT complement each other to solve the problem stated in Equation (1). BO’s ability to rapidly produce candidates and counter-examples initially allows the combination to proceed to maximal regions quickly in most cases while still providing the formal guarantees on the validity and accuracy of stable solutions.
- Figure 1 shows the dependencies between the stability radius and the safety threshold achievable on candidate points. We can observe that initial candidates found by BO are not necessarily stable, and therefore usage of SMT is essential to discover stable solutions.

VII. CONCLUSIONS

We have introduced a hybrid optimization algorithm GEARSAT$_\delta$-BO that uses Bayesian optimization and SMT solvers as its building blocks. SMT solving is used to establish formal guarantees to optimality and stability of the computed solutions. BO on the other hand is used to suggest valuable candidates towards stable near-optimal solutions and significantly speeds up the overall search. In this way we combine the strengths of both approaches: the power of statistical inference by BO to guide the search with formal guarantees provided by SMT.

To the best of our knowledge this is the first work that combines BO and SMT solving to overcome basic limitations...
of the BO, in particular, its inability to give formal guarantees of stability and accuracy of the computed optimum, which becomes possible to resolve in cases when a representation of function is given explicitly rather as a black-box.

We believe that the observation that BO is very good in finding counter-examples in large multi-dimensional spaces, opens up new opportunities for applying BO for counter-example generation and directing the search in multiple areas of automated reasoning and formal verification.

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