

Deciding Predicate Logical Theories of Real-Valued Functions

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Abstract

The notion of a real-valued function is central to mathematics, computer science, and many other scientific fields. Despite this importance, there are hardly any positive results on decision procedures for predicate logical theories that reason about real-valued functions. This paper defines a first-order predicate language for reasoning about multi-dimensional smooth real-valued functions and their derivatives, and demonstrates that—despite the obvious undecidability barriers—certain positive decidability results for such a language are indeed possible.

1 Introduction

Predicate logical decision procedures have become a major workhorse in computer science, for example, as the basic reasoning engines in SAT modulo theory (SMT) solvers [2]. Common decision procedures support theories such as uninterpreted function symbols, arrays, linear integer arithmetic, and real arithmetic. However, many areas of computer science (e.g., computer aided design, formal verification of physical systems, machine learning) use as their basic data structure not only real numbers but real-valued *functions*, for example, to represent solid objects [14], correctness certificates [31, 30] or neural networks [1]. Moreover, due to their fundamental role as a basic mathematical object, real-valued functions are used as a basic modeling tool throughout many further scientific areas. But unfortunately, real-valued functions have been left almost completely untouched by

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research on predicate logical decision procedures. The goal of this paper is to take a first step to fill this gap.

More concretely, the paper provides the following contributions:

- We formalize a first-order language of real-valued functions that allows reasoning about both real numbers and multi-dimensional real-valued smooth functions based on the usual arithmetical operations, function evaluation and differentiation.
- We prove that a quantifier-free fragment of the language that restricts arithmetic to addition and multiplication of real numbers, but still provides function evaluation and differentiation, is decidable.
- We prove that for a fragment of the language that allows arbitrary quantification on real-valued variables (but not on function-valued variables), there is an algorithm that can detect satisfiability for all input formulas that are robustly satisfiable in the sense that there is a satisfying assignment that stays satisfying under small perturbations of the values of function-valued variables.

We neither claim theoretical nor practical efficiency of the resulting decision procedures. Instead, our goal is to overcome scientific fragmentation by developing a framework that can be instantiated to more efficient techniques for specific applications.

The paper has the following structure: In the next section, we discuss related work. In Section 3, we define the syntax and semantics of the mentioned predicate language for reasoning about smooth real-valued functions. In Section 4 we prove decidability of the quantifier-free case. In Section 5 we discuss decidability of the case with arbitrary quantification on real-valued variables. In Section 6 we conclude the paper.

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2 Related Work

Reasoning about real-valued functions—that we also simply call *real functions*—will, of course, be usually based on reasoning about real numbers. This is facilitated by the fact that unlike the case of the integers, in the case of the real numbers, its non-linear theory (i.e., the theory of real closed fields) is decidable [39]. The decidability of the case with the exponential function is still unknown, but is decidable provided Schanuel’s conjecture

holds [26]. Inclusion of the sine function makes the problem undecidable since—as a periodic function—it is able to encode the integers. This makes any theory that allows reasoning about systems of linear ordinary differential equations (ODEs) undecidable, since the sine function appears as the solution of the linear ODE $\dot{x} = -y, \dot{y} = x$.

In mathematical analysis, real functions are often abstracted to elements of abstract function spaces such as Banach spaces and Hilbert spaces [25]. However, with one notable exception [38] we are aware of, corresponding predicate logical decision problems have been largely ignored by computer science.

An important occurrence of real functions is in the role of solutions of ordinary differential equations (ODEs) and hybrid dynamical systems. Formal verification of such systems has been an active research topic over many years [11], with a plethora of decidability and undecidability results [17, 9, 24, 3, 4]. Deductive verification bases formal verification on automated reasoning frameworks such as hybrid dynamic logic [30], or proof assistants such as Isabelle/HOL [16]. Reasoning with functions as the solution of ODEs has been included into SAT solvers without formulation as a first-order decision problem [13, 19]. ODEs have also played a role as objects in constraint programming [22]. In contrast to the work mentioned in this paragraph, in this paper, we introduce a general logical language with variables and predicate and function symbols ranging over real-valued functions. Especially, we allow multi-dimensional functions and partial differentiation, whereas ODEs and hybrid systems are defined using one-dimensional functions, only (the single dimension being time).

Computation in function spaces plays a major role in numerical analysis, where it is mostly restricted to representing solutions to certain specific computation problems, especially, solving ordinary or partial differential equations. There are also some general approaches to computing with functions [12, 10]. However, the basic assumption in numerical analysis is that the solution to the given problem exists and is unique, and the goal is to compute an approximation of this solution, whereas in this paper we consider satisfiability questions, where a proof of existence is the goal, not an assumption.

Computer algebra [42] studies computation with symbolic objects, especially polynomials, that can be interpreted as representations of real functions. Unlike that, in this paper we are interested in solving problems of reasoning about functions that are independent from a certain representation.

Robustness has been recognized as tool for characterizing solvable cases

of undecidable instances of decision problems [17, 33, 18]. However, we are not aware of any work applying this idea to metrics over function spaces.

The proof of decidability of the quantifier-free case will be based on abstracting function variables to uninterpreted function symbols. Abstraction to uninterpreted function symbols is a classical technique in formal verification [5] that has also been applied to real functions [7], but with the goal of modeling *specific* function symbols, while in this paper we are interested in general reasoning about smooth real functions and their derivatives.

3 Formal Syntax and Semantics

In this section, we define the syntax and semantics of the first-order language for reasoning about real functions that we will want to decide. The language will be sorted, allowing variables that range over real numbers and variables that range over real functions. We denote the sort ranging over real numbers, that we also call the *scalar sort*, by \mathcal{R} , and the sorts ranging over real-valued functions, that we also call the *function sorts*, by \mathcal{F}_n , where $n \in \mathbb{N}$ refers to the number of arguments (i.e., dimension of the domain). We will also use the symbol \mathcal{F} to stand for any sort $\mathcal{F}_i, i \in \mathbb{N}$. For each of those sorts, we assume a corresponding set of variables $\mathcal{V} = \mathcal{V}_{\mathcal{R}} \cup \mathcal{V}_{\mathcal{F}_1} \cup \mathcal{V}_{\mathcal{F}_2} \dots$. We will write the elements of $\mathcal{V}_{\mathcal{R}}$ using lower-case letters and the elements of $\mathcal{V}_{\mathcal{F}_1} \cup \mathcal{V}_{\mathcal{F}_2} \dots$ using upper case letters. We will also use the symbol $\mathcal{V}_{\mathcal{F}}$ to denote the set of all function variables $\mathcal{V}_{\mathcal{F}_1} \cup \mathcal{V}_{\mathcal{F}_2} \dots$.

We will build formulas based on the usual syntax of many-sorted first-order logic. Here, we allow rational constants, arithmetical function symbols such as $+$, \times , \exp , \sin , and predicate symbols $=, \leq, \geq, <, >$ that have the usual arity. For every $n \in \mathbb{N}$, we allow the function symbols $app : \mathcal{F}_n \times \mathcal{R}^n \rightarrow \mathcal{R}$ and $\partial_i : \mathcal{F}_n \rightarrow \mathcal{F}_n, i \in \{1, \dots, n\}$ that we call app-operator and differentiation operator, respectively. As usual, we will often write the differentiation operator without parenthesis, and for $X \in \mathcal{F}_1$, we also write \dot{X} instead of $\partial_1 X$. We will also call a term whose outermost symbol is the function symbol app , an *app-term*.

We will call formulas whose function symbols are restricted to $\{+, \times, app\} \cup \{\partial_i \mid i \in \mathbb{N}\}$, and hence avoiding transcendental function symbols, *function-algebraic*. As already mentioned in the introduction, in this paper, we concentrate on this case.

We define the semantics of formulas by defining a structure \mathfrak{A} giving the usual real-valued semantics to all function and predicate symbols. This allows us to avoid questions of axiomatization and, at the same time, ensures

compatibility with applications. Clearly, satisfiability of a formula based on classical mathematical semantics, implies its satisfiability wrt. an arbitrary axiomatization compatible with classical mathematics.

In more detail, the structure \mathfrak{R} will be many-sorted, where the sort \mathcal{R} ranges over the universe of real numbers \mathbb{R} and the sorts $\mathcal{F}_n, n \in \mathbb{N}$ range over the set of smooth (i.e., infinitely often differentiable) functions in $\mathbb{R}^n \rightarrow \mathbb{R}$. We will use the notation that for any smooth function $F : \mathbb{R}^n \rightarrow \mathbb{R}$, and tuple $(\beta_1, \dots, \beta_n) \in \mathbb{N}_0^n$, $D^{(\beta_1, \dots, \beta_n)}F$ denotes the function that is the result of differentiating for every $i \in \{1, \dots, n\}$ the function F β_i -times wrt. its i -th component. The semantics of function and predicate symbols on the real numbers will be as usual. The app-operator and differentiation operator are defined as follows:

- For every $n \in \mathbb{N}$, for all $X \in \mathcal{F}_n$, $\mathfrak{R}(\text{app})(X, x_1, \dots, x_n) = X(x_1, \dots, x_n)$ (i.e., function application in its usual mathematical sense)
- For every $n \in \mathbb{N}$, $i \in \{1, \dots, n\}$, for every $X \in \mathcal{F}_n$, $\mathfrak{R}(\partial_i)(X) = D^d X$, where $d \in \mathbb{N}_0^n$ with $d(i) = 1$ and $d(k) = 0$ (i.e., the result of taking the derivative of X wrt. its i -th argument).

We will denote the set of variable assignments assigning to each variable an element of its respective universe, by \aleph . Given an assignment $\alpha \in \aleph$ we can now assign semantics to formulas in the usual way, writing $\alpha \models \phi$ iff the interpretation given by structure \mathfrak{R} and assignment α satisfies ϕ . We call a formula ϕ *satisfiable* iff there is an assignment $\alpha \in \aleph$ such that $\alpha \models \phi$. In such a case we will also say that ϕ is \mathcal{F} -satisfiable. By abuse of notation, we will use the symbol \mathcal{F} to not only denote the function sorts, but also the *theory* \mathcal{F} of \mathcal{F} -satisfiable formulas.

4 Quantifier-Free Case

In this section, we consider formulas that are quantifier-free and function-algebraic. Here are some examples:

- $\text{app}(X, t) \geq 1 \wedge \text{app}(X, t+1)^2 \leq 1$: This formula restricts the value of the function X at two different points t and $t+1$. Since these points are different, for checking satisfiability of the formula, it suffices check satisfiability of the algebraic inequalities $r \geq 1 \wedge s^2 \leq 1$. Based on a satisfying assignment for this formula, we get a satisfying assignment for the original formula by assigning to X a function interpolating between the values for r and s .

- $app(X, 0) = 0 \wedge app(\dot{X}, 1) = app(X, 1)^2$. This formula not only restricts values for the function X , but also states a relationship between the value of X and its derivative. The formula is satisfiable since the identity function satisfies the properties stated by the formula.
- $app(\partial_1 X, t) = 1 \wedge app(\partial_2 X, t) = 1$. This formula states a relationship between two partial derivatives of X at the same value t . This holds, for example, for the function X with $X(u, v) = u + v$.

The basic idea for deciding such formulas is, that quantifier-free formulas constrain the values of function variables only at a finite (but not fixed) subset of their domain which will allow us to treat them as uninterpreted function symbols. To do so, we have to get rid of the app- and differentiation operators. For this, observe that the only syntactic elements that result in terms of function sort are function variables and differentiation operators. Hence, differentiation operators can only occur in the form of terms of the form $\partial_{i_1} \partial_{i_2} \dots \partial_{i_n} V$. So we let $\tau_\partial(\phi)$ be the formula resulting from replacing every maximal term of this form (i.e., every term of this form that is not an argument of a differentiation operator) by a fresh function variable V_{i_1, \dots, i_n} . For example, $\tau_\partial(app(\partial_1 X, t) + app(\partial_2 X, t) = 1) \equiv app(X_1, t) + app(X_2, t) = 1$.

The next step is to get rid of the app operator. For this, we denote, for every quantifier-free formula ϕ , by $\tau(\phi)$ the result of replacing every app-term $app(X, t_1, \dots, t_k)$ of $\tau_\partial(\phi)$ by $X(t_1, \dots, t_k)$ where in the resulting formula, we now consider X a k -ary function symbol. Continuing the example, we get $\tau(app(\partial_1 X, t) + app(\partial_2 X, t) = 1) \equiv X_1(t) + X_2(t) = 1$.

The resulting formula is formula in the language defined by the combination of the signature of the theory of real-closed fields and the signature of the theory of uninterpreted function symbols. The combination of these two theories, that we will denote by \mathcal{RU} , is decidable: The signatures of the theory of uninterpreted function symbols and the theory of real-closed fields only share equality, and both are stably infinite¹, hence the decision procedures for the individual procedures can be combined to a decision procedure for the combined theory by the Nelson-Oppen theory combination procedure [28, 5]. As a consequence, we can algorithmically decide \mathcal{RU} -satisfiability of translated formulas $\tau(\phi)$. Moreover, the translation preserves satisfiability:

¹A theory T with signature Σ is called stably infinite iff for every quantifier-free Σ -formula ϕ , if F is T -satisfiable, then there exists some T -interpretation that satisfies F and has a domain of infinite cardinality [28, 5].

Theorem 1 *A conjunctive formula ϕ is \mathcal{F} -satisfiable if and only if $\tau(\phi)$ is \mathcal{RU} -satisfiable.*

For proving this theorem, we have to bridge two differences between \mathcal{F} - and \mathcal{RU} -satisfiability: First, the semantics of \mathcal{F} -satisfiability restricts the domain of function variables to specific functions, more concretely, to smooth real function. And second, the theories of real closed fields and uninterpreted function symbols are defined using axioms, unlike our theory \mathcal{F} that we defined semantically, by fixing a certain structure. Before going into the details of the proof, we state a few lemmas. The first one extracts the non-algorithmic core of the Nelson-Oppen method [28, 40, 5]:

Lemma 1 *Let T_1 and T_2 be two stably infinite theories of respective signatures Σ_1 and Σ_2 , having only equality in common. Let ϕ_1 be a conjunctive Σ_1 -formula, and ϕ_2 a conjunctive Σ_2 -formula. Then $\phi_1 \wedge \phi_2$ is $(T_1 \cup T_2)$ -satisfiable iff there is an equivalence relation E on the common variables $V := \text{var}(\phi_1) \cap \text{var}(\phi_2)$ s.t. $\phi_1 \wedge \rho(V, E)$ is T_1 -satisfiable and $\rho(V, E) \wedge \phi_2$ is T_2 -satisfiable, where $\rho(V, E)$ is formula*

$$\bigwedge_{u,v \in V : uEv} u = v \wedge \bigwedge_{u,v \in V : \neg(uEv)} u \neq v.$$

Every $(\Sigma_1 \cup \Sigma_2)$ -formula ϕ can be brought into an equi-satisfiable formula of the form $\phi_1 \wedge \phi_2$, where ϕ_1 is a Σ_1 -formula, and ϕ_2 is a Σ_2 -formula using the so-called variable abstraction phase of the Nelson-Oppen method. In our case, T_1 is the theory of real closed fields, and T_2 the theory of uninterpreted function symbols. For the result

$$X(t) \geq 1 \wedge X(t+1)^2 \leq 1,$$

of translating the first example from the beginning of the section, the result of the variable abstraction phase is the equi-satisfiable formula

$$v_1 \geq 1 \wedge v_2 = t + 1 \wedge v_3^2 \leq 1 \wedge v_1 = X(t) \wedge v_3 = X(v_2).$$

The common variables are $\{v_1, v_2, v_3, t\}$, and the equivalence relation induced by $\{\{v_1, v_3\}, \{v_2\}, \{t\}\}$ illustrates Lemma 1, since $v_1 \geq 1 \wedge v_2 = t + 1 \wedge v_3^2 \leq 1 \wedge v_1 = v_3 \wedge v_1 \neq v_2 \wedge v_3 \neq v_2$ is satisfiable in the theory of real-closed fields, and $v_1 = X(t) \wedge v_3 = X(v_2) \wedge v_1 = v_3 \wedge v_1 \neq v_2 \wedge v_3 \neq v_2$ is satisfiable in the theory of uninterpreted function symbols.

The second lemma states a Hermite-like interpolation property whose proof follows from standard techniques in mathematical analysis.

Lemma 2 *Let p be a function from a finite subset P of $\mathbb{R}^n \times \mathbb{N}_0^n$ to \mathbb{R} . Then there exists a smooth function $F : \mathbb{R}^n \rightarrow \mathbb{R}$ s.t. for every $(x, d) \in P$, $(D^d F)(x) = p(x, d)$.*

Proof. Let X be the set $\{x \mid (x, d) \in P\}$. This set is finite, and hence the elements of X are isolated. For each $c \in X$, construct a function f_c which for all d with $(x, d) \in P$, $(D^d f_c)(x) = p(x, d)$. Let $F = \sum_{c \in X} B_c(f_c)$, where B_c is a smooth function that is equal to the identity function in a sufficiently small neighborhood of c , and zero around all other elements of P (i.e., a so-called bump function). Then F satisfies the desired property. ■

Now we return to the proof of Theorem 1:

Proof. To prove the \Rightarrow direction, we assume a variable assignment α that \mathcal{F} -satisfies ϕ and construct an interpretation that satisfies both the axioms of \mathcal{RU} and the formula $\tau(\phi)$. The interpretation is based on the structure of the real numbers, interprets the symbols $\{0, 1, +, \times, \leq, <, \geq, >\}$ in the usual mathematical way, interprets the function symbols introduced by the translation τ as the corresponding smooth real-valued functions given by α and their respective derivatives, and assigns to the variables of $\tau(\phi)$ the corresponding real values given by α . The result satisfies the formula ϕ by construction and the axioms of \mathcal{RU} since the real numbers are an instance of the theory of real closed fields,

We are left with proving the \Leftarrow direction. For this, we assume that $\tau(\phi)$ is \mathcal{RU} -satisfiable, and build an assignment that satisfies ϕ , assigning to each variable of ϕ an element of the universe of \mathfrak{R} corresponding to its sort (i.e., either a real number and or a smooth real function).

Observe that both the theory of real closed fields and the theory of uninterpreted function symbols are stably infinite. Hence we can apply the Nelson-Oppen method. Let the formulas π_R and π_U be the result of applying the variable abstraction phase of the Nelson-Oppen method to $\tau(\phi)$. Hence, π_R is a formula in the language of real closed fields, and π_U a formula in the language of uninterpreted function symbols s.t. $\pi_R \wedge \pi_U$ is \mathcal{RU} -equi-satisfiable with $\tau(\phi)$. Let V be the common variables of $\pi_R \wedge \pi_U$, and let E be the equivalence relation on V ensured by Lemma 1. Then $\pi_R \wedge \rho(V, E)$ is satisfiable in the theory of real closed fields and $\rho(V, E) \wedge \pi_U$ in the theory of uninterpreted function symbols.

The theory of real closed fields is complete, and hence all its models are elementary equivalent. As a consequence, there is an interpretation I_R that satisfies $\pi_R \wedge \rho(V, E)$ and assigns real numbers to all variables.

Also $\rho(V, E) \wedge \pi_U$ has a satisfying interpretation. However, since the theory of uninterpreted symbols is not complete, we need a more involved construction to come up with an interpretation assigning real numbers and real-valued functions.

We observe that for a formula that is satisfiable in the theory of uninterpreted function symbols, the congruence closure algorithm [29] constructs a satisfying interpretation. Its domain is formed by equivalence classes T_\sim of the set of sub-terms T of the given formula. This domain is finite since the set T is finite. Moreover, each equivalence class contains only finitely many terms. Let I_U be such an interpretation satisfying the formula $\rho(V, E) \wedge \pi_U$. Observe that the arrangement $\rho(V, E)$ ensures that all variables shared by π_R and π_U and belonging to the same equivalence class, must have the same value in I_R .

We will combine the interpretations I_R and I_U into an interpretation I that satisfies $\tau(\phi)$ and, in addition, uses the real numbers as its domain. Hence, we will translate the elements in the domain of I_U to real numbers, and extend them to real-valued functions corresponding to the uninterpreted function symbols.

We will now define a function r assigning to each equivalence class in T_{sim} a distinct real number. Let this function r be such that it assigns to each equivalence class containing a variable shared by π_R and π_U the value of this variable in I_R (as we have observed, this is unique over all such variables belonging to the same equivalence class), and to all other equivalence classes a further, distinct real number. Let $r' : T \rightarrow \mathbb{R}$ s.t. for every term $t \in T$, $r'(t)$ is the real number that r assigns to the equivalence class containing t .

Based on this, let I be the following interpretation which assigns real numbers to all variables in $\tau(\phi)$ and partial real functions to the function symbols in $\tau(\phi)$:

- for every variable x occurring in π_R , $I(x) := I_R(x)$,
- for every variable x occurring in π_U , $I(x) := r'(x)$,
- for every function symbol X of arity k , let $I(X)$ be the partial function such that for every term of the form $X(t_1, \dots, t_k)$ in T , $I(X)(r'(t_1), \dots, r'(t_k)) := r'(X(t_1, \dots, t_k))$, and $I(X)$ is undefined for all other values.

The two following observations make this definition well-formed:

- The first two items overlap. This is no problem since for shared variables, $I(x)$ and $r'(x)$ coincide.

- The definition in the third item is unique since due to the congruence axioms of the theory of free function symbols, for all $t_1, \dots, t_k, t'_1, \dots, t'_k \in T$, $r'(t_1) = r'(t'_1), \dots, r'(t_k) = r'(t'_k)$ implies $r'(X(t_1, \dots, t_k)) = r'(X(t'_1, \dots, t'_k))$.

We will now build a variable assignment α from I such that $\alpha \models \phi$. For every scalar variable x , $\alpha(x) := I(x)$. For every function variable V , $\alpha(V)$ will be a smooth real-valued function whose values coincide with the values of the partial function $I(V)$ on all points where this partial function has a defined value, and whose derivatives coincides with the values of the corresponding partial function $I(V_{i_1, \dots, i_n})$ on all points where the latter has a defined value. Such a function exists due to Lemma 2, and it satisfies the formula ϕ . ■

To illustrate the theorem, we continue with the example from above. The real part of the formula is satisfiable, for example by $\{v_1 \mapsto 1, v_2 \mapsto 7, v_3 \mapsto 1, t \mapsto 6\}$. Applying the congruence closure algorithm to the part with uninterpreted function symbols, we work with the set of sub-terms $T = \{v_1, v_2, v_3, t, X(t), X(v_2)\}$. The result of the congruence closure algorithm is the equivalence relation $\{\{v_1, v_3, X(v_2), X(t)\}, \{t\}, \{v_2\}\}$. Hence $r'(\{v_1, v_3, X(v_2), X(t)\}) = 1, r'(\{t\}) = 6, r'(\{v_2\}) = 7$. However, since every variable in π_U also occurs in π_R , the interpretation I can simply agree with $\{v_1 \mapsto 1, v_2 \mapsto 7, v_3 \mapsto 1, t \mapsto 6\}$ on the real variables. Moreover, it assigns to the function variable X the partial function $\{7 \mapsto 1, 6 \mapsto 1\}$. The corresponding assignment α assigns to the scalar variables the same real values as I , and assigns to X a smooth interpolation of the partial function $\{7 \mapsto 1, 6 \mapsto 1\}$. For example, this could be the constant function that has the value 1, everywhere.

Since a disjunction of formulas is satisfiable, if one of the constituting disjuncts is satisfiable, we get:

Corollary 1 *The quantifier free, function-algebraic theory of real functions is decidable.*

The proof of Theorem 1 also shows how to compute satisfying assignments: After checking the satisfiability of $\tau(\phi)$ using the congruence closure algorithm and the Nelson-Oppen combination procedure, construct the variable assignment α defined in the proof.

Note that the concluding building block of the proof of Theorem 1 is Lemma 2. Any analogous lemma that ensures stronger properties of the constructed functions results in a corresponding strengthening of Theorem 1.

For example, we could also be interested in constructing functions that generalize the constraints given by the input formula as much as possible, maximizing certain regularity properties [15].

5 Scalar Quantification

We will now allow arbitrary quantification on scalar variables. We will still require formulas to be function-algebraic and do not allow quantification on function variables. An example is

$$\forall t \in [0, 10] \exists t' \in [0, 10] . \text{app}(X, t, 2t)^2 + 1 \geq \text{app}(\partial_2 X, t', t'),$$

where $X \in \mathcal{F}_2$ and the interval bounds on variables represent the obvious abbreviations. Many problems resulting from the synthesis of correctness certificates for continuous systems (e.g., Lyapunov function [23], barrier certificates [31] and their generalizations [30, 21]), belong to this class.

In Subsection 5.1 we will introduce a method for proving satisfiability that requires some user-determined choice. In Subsection 5.2 we will introduce a robustness property of formulas that will allow us to characterize solvability of formulas, in Subsection 5.3, to introduce a systematic method to applying the satisfiability check from Subsection 5.1 and ensuring that it will succeed for all formulas satisfying the robustness property. In Subsection 5.4, we will discuss the relevance of the method for practical computation.

5.1 Proving Satisfiability

The method for proving satisfiability that we introduce instantiates function variables to polynomials which will allow us to rewrite the formula into a formula in the language of the theory of real-closed fields which is decidable. In this sub-section, we still assume these polynomials to be given (e.g., chosen by the user), and drop this assumption later.

Definition 1 *We call a function π that assigns to every function variable of sort \mathcal{F}_n a polynomial with rational coefficients in the variables t_1, \dots, t_n a polynomial assignment. Moreover, we call a pair consisting of a formula and a polynomial assignment an instantiated formula.*

The intuition is that the polynomial assignment π in an instantiated formula (ϕ, π) instantiates each function variable in ϕ to the respective polynomial assigned by π . Let us define the following rules on instantiated formulas (ϕ, π) :

Table 1: Polynomial Instantiation

rule	formula	polynomial assignment
	$\forall p \forall q . app(X, q) + p^2 app(\partial_1 X, r) app(Y, q) \geq 0$	$\{X \mapsto t^2 + 1, Y \mapsto t\}$
varsep	$\forall p \forall q . app(X, q) + p^2 app(\partial_1 X', r) app(Y, q) \geq 0$	$\{X \mapsto t^2 + 1, X' \mapsto t^2 + 1, Y \mapsto t\}$
∂ -elim	$\forall p \forall q . app(X, q) + p^2 app(X', r) app(Y, q) \geq 0$	$\{X \mapsto t^2 + 1, X' \mapsto 2t, Y \mapsto t\}$
app-elim	$\forall p \forall q . q^2 + 1 + 2p^2 r q \geq 0$	$\{X \mapsto t^2 + 1, X' \mapsto 2t, Y \mapsto t\}$

- **varsep**: Rename multiple occurrences of the same function variable in ϕ by fresh function variables, and extend π to the new variables in such a way that it assigns the same polynomial to each new variable as to its original one.
- **∂ -elim**: Replace a sub-term of ϕ of the form $\partial_i X$, where X is a function variable, by X and π by π' that is identical to π except that it assigns the result of symbolic differentiation of the polynomial $\pi(X)$ in its i -th argument to the function variable X .
- **app-elim**: Replace a sub-term of ϕ of the form $app(X, \hat{t}_1, \dots, \hat{t}_n)$, where X is a function variable, and the terms $\hat{t}_1, \dots, \hat{t}_n$ do not contain any app-operator, by the result of substituting the values $\hat{t}_1, \dots, \hat{t}_n$ for the respective variables t_1, \dots, t_n in the polynomial $\pi(X)$.

Now apply first the rule varsep, and then iterate applying the elimination rules until they cannot be applied any more. This process must terminate since every application of an elimination rule decreases the total number of ∂ - and app-operators by one. Moreover, the result must be unique since the only possible alternative choices of the rules relate to independent sub-formulas. So denote by $\Pi_\pi(\phi)$ the formula ϕ' where (ϕ', π') is the final result of the described rule-application process.

Table 1 shows the results of the individual steps of the process of forming $\Pi_\pi(\phi)$ for an example of an instantiated formula with $X, Y \in \mathcal{F}_1, p, q, r \in \mathcal{R}$, where the result $\Pi_\pi(\phi)$ can be seen at the bottom of the column “formula”.

Polynomial evaluation completely eliminates any function variables or operators:

Lemma 3 *For every instantiated formula (ϕ, π) , $\Pi_\pi(\phi)$ does not contain any function variable, and hence it also does not contain any app- or diff-operator.*

Proof. Function variables can only occur as arguments to diff and app operators. In such a situation, the rules ∂ -elim and *app*-elim are applicable, and hence, such a formula cannot be the result of $\Pi_\pi(\phi)$. ■

Therefore, if ϕ is function-algebraic, $\Pi_\pi(\phi)$ is a formula in the language of real-closed fields, which is decidable [39]. Moreover, instantiated formulas can be used for proving satisfiability:

Theorem 2 *For every instantiated formula (ϕ, π) , $\pi \models \exists_{\mathcal{R}}\phi$ iff $\Pi_\pi(\phi)$ is satisfiable.*

Proof. For an instantiated formula (ϕ, π) , let $\rho(\phi, \pi)$ be the formula

$$\exists_{\mathcal{R}} \phi \wedge \bigwedge_{X \in \mathcal{V}_F} \forall t_1, \dots, t_n . \text{app}(X, t_1, \dots, t_n) = \pi(X),$$

where $\exists_{\mathcal{R}}$ denotes the existential closure of the formula wrt. the scalar variables (and, strictly speaking, within this formula, $\pi(X)$ is not the polynomial assigned by π to X , but the predicate logical term representing this polynomial).

Now observe that $\pi \models \exists_{\mathcal{R}}\phi$ iff $\rho(\phi, \pi)$ is satisfiable. Moreover, every element of the sequence $\rho(\phi_1, \pi_1), \dots, \rho(\phi_n, \pi_n)$ with $(\phi_1, \pi_1) = (\phi, \pi)$, $\phi_n = \Pi_\pi(\phi)$, and each (ϕ_i, π_i) , $i \in \{2, \dots, n\}$ being the result of the application of a rewrite rule to (ϕ_{i-1}, π_{i-1}) , is equi-satisfiable. Finally $\rho(\phi_n, \pi_n)$ and $\phi_n = \Pi_\pi(\phi)$ are equi-satisfiable since $\Pi_\pi(\phi)$ does not contain any function variable. ■

So we have reduced the satisfiability checking problem to the problem of finding a polynomial assignment π for which $\Pi_\pi(\phi)$ is satisfiable. However, for some formulas, this is bound to fail, which can be easily seen on the simple initial value problem

$$\text{app}(X, 0) = 1 \wedge \forall t . t \geq 0 \Rightarrow \text{app}(\dot{X}, t) = \text{app}(X, t)$$

that is satisfiable, but not by any polynomial assignment (the only solution of the given initial value problem is the exponential function).

5.2 Robust Satisfiability

Even though differential equations such as $\dot{x} = x$ (in our notation: $\forall t . \text{app}(\dot{X}, t) = \text{app}(X, t)$) are ubiquitous in mathematics, they are highly idealized objects:

In practice, no real physical system will satisfy such an equation precisely, and concrete differential equations can only be used in applications after introducing many simplifying assumptions that are part of the daily bread of practical engineering. However, this also makes it necessary for engineers to assess the consequences of such simplifications. Despite the existence of powerful deductive verification techniques [30, 16], in practice, differential equations are still solved by algorithms [20] that produce approximation errors both due to discretization and due to floating point computation. The reliability of the whole process depends essentially on the fact that the error made by the solver does not dominate the error made by simplifying assumptions. This is a major complication, that could be avoided if solvers could conservatively bound the produced errors. For the concrete example $\dot{x} = x$, it would be very useful, if a solver could—instead of solving the differential equation approximately—guarantee the solution of $x - \epsilon \leq \dot{x} \leq x + \epsilon$ within a compact set, for a small constant $\epsilon > 0$. In this section, we will formally characterize such situations and show that in such cases, a formally correct satisfiability check is not only possible, but that we can even guarantee its success.

For being able to measure the distance between variable assignments, we will adjoin metrics to the set of variable assignments \aleph , making the pair (\aleph, d) a metric space. These metrics will be parametric in a family of compact sets $K_n \subseteq \mathbb{R}^n, n \in \mathbb{N}$ which we will call *domain of interest*. We will denote this dependence on the domain of interest by an index, writing d_K for the metric associated to domain of interest K . We will call such a metric on \aleph a *variable assignment metric*.

Definition 2 *A formula ϕ is semantically robustly satisfiable wrt. a variable assignment metric d iff there is a variable assignment $\alpha \in \aleph$ and an $\epsilon > 0$ (that we call the robustness margin) such that for every α' with $d_K(\alpha, \alpha') < \epsilon$, $\alpha' \models \phi$.*

Note that unlike similar definitions [18, 34], this definition only depends on the semantics of a given formula, but not on its syntax, and hence is invariant wrt. equivalence transformations. We will later see that this is made possible by the fact that we restrict ourselves to operations on real numbers allowed by the decidable theory of real closed fields.

We will usually use metrics induced by some norm, and so we will call a formula robustly satisfiable wrt. a norm $\|\cdot\|_K$ iff it is robustly satisfiable wrt. the metric $d_K(x, x') = \|x - x'\|_K$. Given metrics $d^{\mathcal{T}}$ on \mathcal{T} , where $\mathcal{T} \in \{\mathcal{R}, \mathcal{F}_1, \dots\}$, we define their extension to variable assignments element-

wise. So, for $\alpha, \alpha' \in \aleph$,

$$d_K(\alpha, \alpha') := \max_{\mathcal{T} \in \{\mathcal{R}, \mathcal{F}_1, \dots\}} \max_{v \in \mathcal{V}_{\mathcal{T}}} d_K^{\mathcal{T}}(\alpha(v), \alpha'(v)).$$

Here, we will usually use a family of metrics on function variables of all dimensions. If $d^{\mathcal{R}}$ is a metric on \mathbb{R} and $d^{\mathcal{F}}$ such a family of metrics on smooth functions $\mathbb{R}^i \rightarrow \mathbb{R}, i \in \mathbb{N}$, then we will denote this extension to variable assignments by $d^{\mathcal{R}} \times d^{\mathcal{F}}$.

On real-numbers we will use the discrete metric $d^=(x, y) := \begin{cases} 1, & \text{if } x \neq y, \\ 0, & \text{if } x = y. \end{cases}$

The metric on functions will be based on a norm measuring the size of a given function and of its derivatives. For a function $F : \mathbb{R}^n \rightarrow \mathbb{R}$, at least k -times differentiable, let

$$\|F\|_K^k := \max_{|\beta| \leq k} \inf_{x \in K_n} |(D^\beta F)(x)|.$$

We denote the metric induced by this norm $\|\cdot\|_K^k$ by d_K^k . Here are some examples:

- $\forall t \in [0, 1] . app(X, t) - 0.1 \leq app(\dot{X}, t) \wedge app(\dot{X}, t) \leq app(X, t) + 0.1$, with $x \in \mathcal{F}_1$ is *not* robustly satisfiable wrt. the norm $\|\cdot\|_{[0,1]}^0$, since that norm does not constrain any derivative of x . However, it is robustly satisfiable wrt. $\|\cdot\|_{[0,1]}^1$, since every function with maximal distance 0.01 from the exponential function wrt. $\|\cdot\|_{[0,1]}^1$ satisfies the formula.
- $\forall t \in [0, 1] . app(\dot{X}, t) = app(X, 0)$ is not robustly satisfiable wrt. $\|\cdot\|_{[0,1]}^0$, since for every function satisfying the formula adding the term et to the function results in a function not satisfying it.
- The formula $\forall t . app(X, t) \geq 0$, while satisfiable, is not robustly satisfiable wrt. the norm $\|\cdot\|_{[0,1]}^0$, since this norm only restricts the value of functions in the domain of interest $[0, 1]$. Due to this, for every variable assignment α satisfying the formula, there is an α' with $d(\alpha, \alpha') = 0$ that does not satisfy the formula: Simply choose an α' that is identical to α on $[0, 1]$ but reaches a negative value outside of this interval. In contrast to that, the formula $\forall t \in [0, 1] . app(X, t) \geq 0$, is robustly satisfiable which explains the importance of bounds on quantified variables for ensuring robustness.

5.3 Robust Completeness

We will now introduce a systematic method that checks satisfiability using the test from Subsection 5.1 and that will succeed for all formulas satisfying the robustness property from Subsection 5.2. We will use the fact that one can approximate smooth functions on compact domains arbitrarily closely by polynomials. For this, recall that a subset X' of a metric space (X, d) is dense in (X, d) iff for every $x \in X$ and $\varepsilon > 0$ there is an $x' \in X'$ with $d(x, x') < \varepsilon$.

Lemma 4 *Let ϕ be a formula, d a variable assignment metric and $\aleph' \subseteq \aleph$ s.t. \aleph' is dense in (\aleph, d) . Then every formula that is semantically robustly satisfiable wrt. the metric d has a satisfying assignment from \aleph' .*

Proof. Assume that ϕ is semantically robustly satisfiable wrt. d . Then there is a variable assignment $\alpha \in \aleph$ and an $\varepsilon > 0$ such that for every α' with $d(\alpha, \alpha') < \varepsilon$, $\alpha' \models \phi$. Since \aleph' is dense in (\aleph, d) , there is an $\alpha' \in \aleph'$ with $d(\alpha, \alpha') < \varepsilon$. Hence α' is within the robustness margin of α , and hence $\alpha' \models \phi$.

Now we observe:

Lemma 5 *For every $k \in \mathbb{N}_0$, compact $K \subseteq \mathbb{R}^n$, the set of n -dimension polynomial functions with rational coefficients is dense in the set of n -dimensional polynomial functions with real coefficients wrt. the metric d_K^k .*

Proof. Let P be a polynomial function with real coefficients and $\varepsilon > 0$. We will prove that there is a polynomial P' with rational coefficients such that $d_K^k(P, P') < \varepsilon$, that is $\max_{|\beta| \leq k} \inf_{x \in K} |(D^\beta P)(x) - (D^\beta P')(x)| < \varepsilon$. During this, we will separate any given polynomial P into its vectors of coefficients C_P and monomials M_P . Hence $P = C_P^T M_P$.

Let $m = \max_{|\beta| \leq k} \inf_{x \in K} \|M_{D^\beta P}(x)\|$ with $\|\cdot\|$ denoting the Euclidean metric. The value m is finite since K is compact. Let P' be a polynomial with rational coefficients s.t. $M_P(x) = M_{P'}(x)$ and s.t. $\|(C_{D^\beta P} - C_{D^\beta P'})^T\| < \frac{\varepsilon}{m}$. Now, due to Cauchy-Schwarz,

$$\begin{aligned} \max_{|\beta| \leq k} \inf_{x \in K} |(D^\beta P)(x) - (D^\beta P')(x)| &= \max_{|\beta| \leq k} \inf_{x \in K} |(C_{D^\beta P} - C_{D^\beta P'})^T M_{D^\beta P}(x)| \leq \\ &\max_{|\beta| \leq k} \inf_{x \in K} \|M_{D^\beta P}(x)\| \|(C_{D^\beta P} - C_{D^\beta P'})^T\| < m \frac{\varepsilon}{m} = \varepsilon \end{aligned}$$

■

Moreover, the classical Stone-Weierstrass theorem generalizes to d_K^k , that is, the polynomials with real coefficients $P(\mathbb{R})$ are dense in the set of C_k -real functions on any compact set K wrt. d_K^k [41, 27]. This allows us to conclude:

Lemma 6 *For every $k \in \mathbb{N}_0$ and compact $K \subseteq \mathbb{R}^n$, the set of n -dimensional polynomial functions with rational coefficients is dense in the metric space (\aleph, d_K^k) .*

Putting everything together, we get:

Theorem 3 *For every $k \in \mathbb{N}_0$ and a family of compact sets $K_n \subseteq \mathbb{R}^n$, $n \in \mathbb{N}$, there is an algorithm for checking satisfiability of function-algebraic formulas that terminates for every input formula that is semantically robustly satisfiable wrt. the metric $d^\# \times d_K^k$.*

Proof. Assume a semantically robustly satisfiable function-algebraic formula ϕ . Since by Lemma 6, the set of variable assignments assigning real values to scalar variables and polynomials with rational coefficients to function variables is dense in the metric space $(\aleph, d^\# \times d_K^k)$, by Lemma 4, there is an assignment $\alpha \in \aleph$ that assigns polynomials with rational coefficients to function variables and that satisfies ϕ . The restriction of α to a polynomial assignment α_π satisfies $\exists_{\mathcal{R}}\phi$.

Due to Theorem 2 we can algorithmically check whether for a given polynomial assignment π , $\pi \models \exists_{\mathcal{R}}\phi$. Moreover, the set of polynomial assignments is recursively enumerable. Hence, an algorithm that enumerates its elements, checking for each element π whether $\Pi_\pi(\phi)$ is satisfiable in the theory of real closed fields, will eventually find α_π , and hence terminate proving that ϕ is satisfiable. ■

Note however, that we do not know how to check a given formula for robustness. Hence, for a given formula we do not know a-priori whether the enumeration algorithm from the proof of Theorem 3 will terminate. We just know that will terminate *under the assumption* that the formula is robust.

5.4 Practical Computation—Templates

Of course, the algorithm from the proof of Theorem 3 is hopelessly inefficient in practice. Still, our approach may provide useful practical insight. In practice, problems of the kind studied here are solved in many, often distant areas [37, 32, 35, 36]. A common approach is to restrict the set of potential

solutions to a fixed class of functions given by a parameterized expression (sometimes also called a *template*), and then searching for values for the parameters such that the result of instantiating the parameters by those values represents a solution to the problem.

There are two main classes of templates that are often used here. The first class are templates given by complex expressions, often called neural networks. The second class are polynomials whose coefficients are parameters which allows many methods to exploit the fact that polynomials are linear in their coefficients. If the given template polynomial does not represent a solution, one can increase the degree of the polynomial. The resulting loop amounts to an enumeration of all polynomials with real coefficients. Our approach (1) formally justifies such algorithms showing that such a loop must terminate for all robust inputs, and (2) generalizes such algorithms to all formulas belonging to the language used in this paper.

6 Conclusion

We have developed a framework for decision procedures for a predicate logical theory formalizing a notion that is central to mathematics, computer science, and many other scientific fields—real-valued functions. Our long-term vision is to replace the need for research on application-specific automated reasoning techniques for smooth real-valued functions by a common framework that results in tools that can be used out-of-the-box in a similar way as decision procedure for common first-order theories in the frame of SMT solvers [2].

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