Specification Construction Using Behaviors, Equivalences, and SMT Solvers

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***Abstract*—We propose a method to write and check a specification including *quantifiers* using behaviors, i.e., input-output pairs. Our method requires the following input from the user: (1) answers to a finite number of queries, each of which presents some behavior to the user, who responds informing whether the behavior is "correct" or not; and (2) an "equivalence" theory (set of formulae), which represents the users opinion about which pairs of behaviors are equivalent with respect to the specification; and (3) a "vocabulary," i.e., a set of formulae which provide the basic building blocks for the specification to be written. Alternatively, the user can specify a type theory and a simple relational grammar, and our method can generate the vocabulary and equivalence theories. Our method automatically generates behaviors using a *satisfiability modulo theory* solver.**

Since writing a specification consists of formalizing ideas that are initially informal, *there must, by definition, be at least one "initial" step where an informal notion is formalized by the user in an ad hoc manner.* This step is the provision of the equivalence theory and vocabulary; we call it the *primitive formalization step*.

We contend that it is considerably easier to write an equivalence theory and vocabulary than to write a full-blown formal specification from scratch, and we provide experimental evidence for this claim. We also show how vocabularies can be constructed hierarchically, with a specification at one level providing vocabulary material for the next level.

I. Introduction

The derivation of programs from formal specifications, and the construction of a correctness proof hand-in-hand with the program has been advocated by Dijkstra [9], Hoare [19], Gries [14], and others. Central to this method is the a priori existence of a formal specification which is assumed to represent what the user requires. The task of constructing such a specification is addressed by the many requirements elicitation methods appearing in the literature [16], [15], [17], [21], [7], [11], [18], [23], [13], [22], and is recognized to be the most crucial part of the software life cycle, as Brooks notes in [6]:

> The hardest single part of building a software system is deciding precisely what to build. No other part of the conceptual work is so difficult as establishing the detailed technical requirements, including all the interfaces to people, to machines, and to other software systems. No other part of the work so cripples the resulting system if done wrong. No other part is more difficult to rectify later.

We aim to ameliorate the difficulty of one crucial part of this problem: writing a functional specification for a single procedure. We present a method for the construction of quantified formal specifications for transformational, terminating, sequential programs. Our method automatically constructs a specification, using the results from a finite number of queries to the user, which the user answers interactively.

Our method relies on an underlying type theory τ, which defines the data types over which the specification is written. A specification $\mathcal{S} = (P, Q)$ consists of a precondition, postcondition pair, written in first order logic. There is a single input σ_i, which is restricted by the precondition P, and a single output σ_o, which is related to the input by the postcondition Q. A specification is satisfied iff the precondition (evaluated on the input) implies the postcondition (evaluated on the input and the output). The pair $\sigma = (\sigma_i, \sigma_o)$ is called a behavior, and we write $\sigma \models \mathcal{S}$ iff $P(\sigma_i) \Rightarrow Q(\sigma_i, \sigma_o)$. We also say that the behavior is correct w.r.t. the specification.

The problem we address is *specification construction*: to write a specification which accurately reflects the users *intentions*. But how are these intentions to be expressed? We express the users intentions as the answers to a sequence of queries of the form: "is the behavior $\sigma_i = \ldots$, $\sigma_o = \ldots$ a correct behavior?" Here the ... represent the actual variable values defined by σ_i, σ_o. Thus, the user identifies those behaviors which the specification (that is being constructed) must admit as correct. After a sufficient number of answers to such queries, our algorithm produces a specification which accurately reflects the intentions of the user. We make precise in the sequel this notion of an accurate specification.

In practice, it is easier to produce the precondition and the postcondition separately, and so we reduce the problem of writing a specification (a pair of predicates) to the problem of writing a single predicate, which we call the *formula construction* problem.

Let Σ be the set of all possible behaviors. The formula construction problem is to write a first-order formula $\mathcal{F}$ that accurately reflects the intentions of the user. We take the users intentions to be a partition $\{vtt, vff\}$ of Σ, where vtt are the behaviors for which $\mathcal{F}$ should evaluate to true, and vff are the behaviors for which $\mathcal{F}$ should evaluate to false. The user expresses this intention as the answers to a sequence of queries of the form: "is the behavior $\sigma_i = \ldots$, $\sigma_o = \ldots$ a behavior for which $\mathcal{F}$ should evaluate to $true$? (i.e., in vtt?) That is, the user serves as an oracle, and determines for each behavior $\sigma = (\sigma_i, \sigma_o)$ that our algorithm presents in a query, whether $\sigma \in vtt$ or not. $\mathcal{F}$ is then constructed as the disjunction of all the σ that are in vtt, where each $\sigma$is converted to a formula in the obvious manner. The problem is that Σ is infinite in general, so we need an infinite number of queries to the user, and the resulting $\mathcal{F}$ is infinitely long. We reduce the number of queries, and the length of $\mathcal{F}$, to finite, by partitioning Σ into a finite number of subsets (equivalence classes) such that all the σin each class have the same classification with respect to whether they are in vtt or in vff. We then query the user with one representative from each class, and construct $\mathcal{F}$ as the disjunction of all cases that the user classifies in vtt.

Consider a first order theory γ, i.e., a countable set of first order wff's. Two elements of Σ are equivalent with respect to γ iff they assign the same truth values to all the formulae in γ. Let Σ/γ denote the resulting partition of Σ. Our goal is to work within a finite partition of Σ, which results from using a finite set of wff's.

Initially, we have available the underlying type theory τ, which defines the data types over which the specification is written. This is usually a countable set of wff's. We next define an equivalence theory ε, also a countable set of first order wff's. The meaning of ε is that two behaviors in the same class of Σ/ε are "the same" with respect to the problem being specified. For example, if the problem is sorting, then two input arrays are "the same" iff corresponding pairs of elements in both arrays have the same ordering. We provide an algorithm to deduce a finite version ε_b of ε, for use in the formula construction algorithm. Although ε_b is finite, using it directly results, in general, in impractically long formulae since Σ/ε_b, while finite, is too large. To improve the succinctness of the constructed formula $\mathcal{F}$, and also to enable a hierarchical methodology, we introduce the notion of vocabulary ν, which is a finite set of wff's, and which induces a coarser partition Σ/ν than Σ/ε_b. $\mathcal{F}$ is written using the formulae in ν. The number of queries to the user that are needed is bounded by $|\Sigma/\nu|$, the number of equivalence classes in Σ/ν.

Now $\mathcal{F}$ must express $\{vtt, vff\}$ in that $\{\sigma \mid \sigma \models \mathcal{F}\}$ = vtt, i.e., $\mathcal{F}$ evaluates to true *exactly* on the behaviors in vtt. This requires that if $\mathcal{F}$ holds for some representative of some class in Σ/ν, that it must then hold for all elements in that class. For this to be possible, no class in Σ/ν can have elements in both vtt and in vff. That is, Σ/ν must be finer than $\{vtt, vff\}$. This property is called *adequacy* of the vocabulary. For example, the vocabulary $\{a[i] \leqslant a[i+1]\}$ is inadequate to specify sorting, since it does not enable the expression of the permutation condition: its equivalence partition is too coarse. We provide algorithms to both construct the formula $\mathcal{F}$ for $\{vtt, vff\}$ given an adequate vocabulary, and also to check if a vocabulary ν is adequate, given an equivalence theory ε and user answers to vtt/vff classification queries. Our algorithm augments an inadequate vocabulary to make it adequate by adding some more formulae.

Since each of τ, ε, and ν is written using formulae from the previous theory, Σ/τ, Σ/ε, and Σ/ν form an increasingly coarser sequence of partitions of Σ.

In practice τ, ε and ν come from (1) the user directly, (2) from existing specifications and code elements, or (3) from syntax rules restricting τ to a finite index theory. In the latter case, ε and adequacy can be computed while computing $\mathcal{F}$.

II. Preliminaries: behaviors and specifications

We use (unless otherwise stated) many-sorted first-order logic [10, Chapter 4]. We use a first order language with both global and local symbols. The global symbols are (1) the boolean connectives and equality (=); (2) n-ary predicate symbols ($n \geqslant 0$); and (3) n-ary function symbols ($n \geqslant 0$). The local symbols are the variables.

We are interested in writing specifications for terminating sequential programs, which have a fixed set $x_1, \ldots, x_n$ of program variables, which take values from universes $U_1, \ldots, U_n$, respectively. A *specification* then consists of a precondition over the initial values of $x_1, \ldots, x_n$, and a postcondition that relates the initial and final values of $x_1, \ldots, x_n$.

Hence we introduce logical variables $x^i_1, \ldots, x^i_n$ for the initial values of the $x_1, \ldots, x_n$, and logical variables $x^o_1, \ldots, x^o_n$ for the final values of the $x_1, \ldots, x_n$. These will be the only variables in our first order language. An input state $\sigma_i : \langle x^i_1, \ldots, x^i_n \rangle \to U_1 \times \cdots \times U_n$ is an assignment that maps each x^i_j, $j \in [1 : n]$, to a value in its domain, and similarly for an output state $\sigma_o : \langle x^o_1, \ldots, x^o_n \rangle \to U_1 \times \cdots \times U_n$. A behavior $\sigma = (\sigma_i, \sigma_o)$ is a pair consisting of an input state and an output state.

A formula is interpreted in a many-sorted structure (I, σ), with a universes $U_1, \ldots, U_n$. I provides the interpretation for the global symbols, and σ provides the interpretation for the local symbols, i.e., the $x^i_1, \ldots, x^i_n, x^o_1, \ldots, x^o_n$. I provides the usual interpretations of functions and relations over the integers, etc. Let f be a well-formed formula (wff). We write $(I, \sigma) \models f$ iff f is true in the structure (I, σ), according to the usual Tarskian semantics. We usually omit I, as it is fixed, and write $\sigma \models f$. We also write $\sigma.f$ for the truth value of f in (I, σ). $[f]$ denotes $\{\sigma \mid \sigma \models f\}$, i.e., the set of states where f holds.

A *specification* $\mathcal{S} = (P, Q)$, consists of two well-formed formulae: P which represents the precondition, and is restricted to contain only $x^i_1, \ldots, x^i_n$, and Q, which represents the postcondition. A behavior $\sigma = (\sigma_i, \sigma_o)$ *satisfies* a specification $\mathcal{S} = (P, Q)$ iff $\sigma.(P \Rightarrow Q) = true$. We write $\sigma \models \mathcal{S}$ in this case, and $\sigma \not\models \mathcal{S}$ otherwise. We also write $[\mathcal{S}] \triangleq \{\sigma \mid \sigma \models \mathcal{S}\}$.

Let Σ be the set of behaviors. We partition Σ into:

- `good`, the set of good (positive) behaviors: the precondition holds before and the postcondition holds after, i.e., $\sigma.P = true$ and $\sigma.Q = true$ for all $\sigma \in$ `good`;
- `bad`, the set of bad (negative) behaviors: the precondition holds before and the postcondition does not hold after, i.e., $\sigma.P = true$ and $\sigma.Q = false$ for all $\sigma \in$ `bad`; and
- `dontCare`, the set of don't care behaviors: the precondition does not hold before, and the postcondition can be either true or false after, i.e., $\sigma.P = false$ for all $\sigma \in$ `dontCare`.

A partition (`good`, `bad`, `dontCare`) of Σ is *feasible* iff (1) for every input state σ_i, there do not exist two output states $\sigma_o, \sigma_{o'}$ such that $(\sigma_i, \sigma_o) \in$ `good` $\cup$ `bad` and $(\sigma_i, \sigma_{o'}) \in$ `dontCare`); and (2) for every input state σ_i there exists an output state σ_o such that $(\sigma_i, \sigma_o) \in \texttt{good} \cup \texttt{dontCare}$). Clause (1) means that the precondition is not both true ($(\sigma_i, \sigma_o) \in \texttt{good} \cup \texttt{bad}$) and false ($(\sigma_i, \sigma_{o'}) \in \texttt{dontCare}$) when evaluated on input σ_i. Clause (2) means that for every input there is at least one acceptable output. In the sequel, we consider only feasible partitions of Σ. We assume that the developer can reliably classify given behaviors as good, bad, and dontCare behaviors.

III. The Specification and Formula Construction Problems

Definition 1 (Specification construction problem): Let $(\texttt{good}, \texttt{bad}, \texttt{dontCare})$ be a feasible partition of Σ. The *specification construction problem* is to find a specification $\mathcal{S}$ such that $[\mathcal{S}] = \texttt{good} \cup \texttt{dontCare}$.
We say that such an $\mathcal{S}$ is *accurate* with respect to $(\texttt{good}, \texttt{bad}, \texttt{dontCare})$.

Definition 2 (Formula construction problem): Let (vtt, vff) be a partition of Σ. The *formula construction problem* is to find a wff $\mathcal{F}$ such that $[\mathcal{F}] = vtt$.
We say that such a $\mathcal{F}$ is *accurate* with respect to (vtt, vff).
We reduce specification construction to formula construction, as follows. Construct a formula P that is accurate w.r.t. $(\texttt{good} \cup \texttt{bad}, \texttt{dontCare})$. Also construct a formula Q that is accurate w.r.t. $(\texttt{good} \cup \phi, \texttt{bad} \cup \psi)$, where (ϕ, ψ) is an arbitrary partition of $\texttt{dontCare}$, which can be chosen for convenience of expressing Q. From the definitions of $\sigma \models \mathcal{S}$ and $[\mathcal{S}]$ given above, we obtain $[\mathcal{S}] = \texttt{good} \cup \texttt{dontCare}$, and so $\mathcal{S}$ is accurate with respect to $(\texttt{good}, \texttt{bad}, \texttt{dontCare})$.

IV. The Formula Construction Algorithm

Let F be a set of first order wff's. $V : F \to \{tt, ff\}$ is a *valuation of* F, i.e., a mapping that assigns to each $f \in F$ a truth-value. Write $F \mapsto \{tt, ff\}$ for the set of valuations of F. Define $fm(V) \triangleq (\wedge f \in F : f \equiv V.f)$, i.e., $fm(V)$ is the formula which asserts that each $f \in F$ has the truth value assigned to it by V. $fm(V)$ can be infinitely long, i.e., it is a formula of the infinitary logic $L_{\omega_1,\omega}$ [2]. Define $[V] \triangleq \{\sigma \mid \sigma \in \Sigma \wedge (\wedge f \in F : \sigma.f = V.f)\}$, i.e., $[V]$ is the set of all behaviors that assign the same values to the formulae in F that V does. Note that $[V] = [fm(V)]$. $F_\sim = \{\langle \sigma, \sigma' \rangle \mid (\wedge f \in F : \sigma.f = \sigma'.f)\}$ is the equivalence relation on Σ that considers two elements equivalent iff they assign the same values to the formulae in F. Thus $\Sigma / F_\sim = \{[V] \mid V \in F \mapsto \{tt, ff\}\}$ is a partition of Σ. We assume the standard definitions for one partition of Σ being finer (coarser) than another, and write $\Sigma/E \leqslant \Sigma/E'$ when Σ/E is finer than Σ/E'.

A. Type theory, equivalence theory, and vocabulary

Our solution to the formula construction problem rests on three foundations: (1) the use of an underlying *type theory* τ, which defines the domains of all the free variables, and also all the operators over these variables; and (2) the use of an *equivalence theory* ε, which defines an equivalence relation over Σ; and (3) the use of a *vocabulary* ν for constructing our formula $\mathcal{F}$. All of these are sets of first order wff's.

1) Type theory: The type theory τ represents the "finest granularity of expression" that we have. It provides the basic axioms for all the free variables, e.g., integer scalars, array indices, arrays, etc. See for example, [4] for an example array theory, and [12] for an example theory of sequences. In practice, the type theory is supported by the SMT solver.

2) Equivalence theory: The user is required to provide the equivalence theory ε as the **primitive formalization step**. Two behaviors that induce the same valuations of all formulae in ε are considered equivalent: $\sigma \equiv_\varepsilon \sigma' \triangleq (\forall\, f \in \varepsilon : \sigma.f = \sigma'.f)$, which can also be written $\sigma \equiv_\varepsilon \sigma' \triangleq (\exists\, V_\varepsilon : \sigma \in [V_\varepsilon] \wedge \sigma' \in [V_\varepsilon])$. Thus, ε represents the users opinion of which parts of Σ will be considered equivalent with respect to the problem being specified. We illustrate with two examples:

- search of an array a between indices ℓ and r inclusive:
  - $\{|a| = n \text{ for all } n > 0\}$
  - $\ell = r$, $\ell < r$
  - $\ell \geqslant 0$, $\ell \leqslant |a| - 1$, $\{\ell = c \text{ for all } c \text{ such that } 0 \leqslant c < |a|\}$
  - $r \geqslant 0$, $r \leqslant |a| - 1$, $\{r = c \text{ for all } c \text{ such that } 0 \leqslant c < |a|\}$
  - $\{a[i] = e \text{ for all } i \text{ such that } 0 \leqslant i < |a|\}$
  - $\{rv = c \text{ for all } c \text{ such that } 0 \leqslant c < |a|\}$
  - $rv = -1$

  That is, values for the left bound ℓ, are equivalent iff either they are equal or they are both out of bounds in the same manner (too low, too high). Likewise for the right bound r. Values for the array a are equivalent iff they are the same size and corresponding elements are equivalent w.r.t. matching the search expression e. Values for the return index rv are equivalent if they are both -1, or they both indicate the same position in the array.
- sort an array a :
  - $\{|a| = n \text{ for all } n > 0\}$
  - $\{a[i] < a[j] \text{ for all } i, j \text{ such that } 0 \leqslant i < j < |a|\}$
  - $\{a[i] = a[j] \text{ for all } i, j \text{ such that } 0 \leqslant i < j < |a|\}$

  That is, values for array a are equivalent iff they are the same size and corresponding pairs of elements have the same order and equality relationship.

We express an equivalence theory using both single formulae, e.g., $\ell = r$, and sets of formulae, e.g., $\{\ell = c \text{ for all } c \text{ such that } 0 \leqslant c < |a|\}$. For now we assume that ε is a finite set of wff's, and so, e.g.,, we restrict $|a|$ to a finite value. We show in Section VI how to deal with equivalence theories consisting of a countable set of wff's.

We argue that equivalence is a notion that is intuitively well understood informally, and is moreover relatively easier to formalize than a complete specification. We justify this claim by a series of examples: since the claim is inherently informal, it can be supported only by empirical evidence.

ε provides an initial set of wff's that are "building blocks" for the formula $\mathcal{F}$ that we are constructing. We cannot use τ directly for this, since the number of formulae that must be considered is infinite, in general, and so we have computability limitations. Since τ is our basic vocabulary, all formulae of ε are written using formulae in τ. Hence we immediately obtain:

Proposition 1: $\Sigma/\tau \leqslant \Sigma/\varepsilon$

To be able to express $\{vtt, vff\}$ using ε, we assume the following axiom:

$$\Sigma/\varepsilon \leqslant \{vtt, vff\} \qquad \text{Axiom-E}$$

That is, we consider only partitions $\{vtt, vff\}$ that are coarser that Σ/ε. This is reasonable, since the number of partitions of Σ is usually uncountable (when the input and output variables are boolean, string, and integer), while the number of formulae that we can write is countable (assuming that the number of variables, and function and predicate symbols, is countable). Hence some restriction on the partitions that can be expressed is required. Also, ε defines the pairs of valuations σ, σ' that the user considers equivalent. Thus any predicate that the user wishes to define must take the same values on σ and σ'. So, $\mathcal{F}$ must correspond to partitions coarser than Σ/ε. This is reasonable, since ε is the first formalization step, and so defines in effect the formal elements from which $\mathcal{F}$ is written.

We emphasize that the *only* requirement on ε is Axiom-E, and so writing ε is easier than writing a full and accurate specification from scratch.

3) Vocabulary: By Axiom-E, each $[V_\varepsilon]$ is wholly contained in either vtt or in vff. Hence the union of all V_ε that are contained in vtt is exactly vtt: $vtt = (\bigcup V_\varepsilon : [V_\varepsilon] \subseteq vtt : [V_\varepsilon])$. Hence, the disjunction of all the formulae $fm(V_\varepsilon)$ corresponding to V_ε that are contained in vtt yields a formula which is true at all elements of vtt and false outside of vtt. That is, $\mathcal{F} = (\bigvee V_\varepsilon : [V_\varepsilon] \subseteq vtt : fm(V_\varepsilon))$. is a tentative solution to the formula construction problem since $[f] = vtt$. However, in practice, this solution is far too verbose to be useful, since the number of equivalence classes in Σ/ε is far too large, each such class consisting of all valuations that the user considers "equivalent" w.r.t. the specific problem being solved. The vocabulary ν introduces the coarser building blocks needed to write $\mathcal{F}$ succinctly. Its formulae are constructed from those of ε, and so we have:

Proposition 2: $\Sigma/\varepsilon \leqslant \Sigma/\nu$

by construction of ν. To be able to express $\{vtt, vff\}$ using ν, we require

$$\Sigma/\nu \leqslant \{vtt, vff\} \qquad \text{(Ad)}$$

that is, $(\forall V_\nu : [V_\nu] \subseteq vtt \vee [V_\nu] \subseteq vff)$. We call such a ν *adequate*. Unlike the situation for ε, we cannot take $\Sigma/\nu \leqslant \{vtt, vff\}$ as an axiom, since ν can contain arbitrarily coarse formulae, i.e., formulae f with large $[f]$. In practice, we wish to use the coarsest formulae possible, since this will give the most succinct expression of $\{vtt, vff\}$. So often, Σ/ν will be too coarse, violating $\Sigma/\nu \leqslant \{vtt, vff\}$, and will have to be corrected. A heuristic for writing an adequate vocabulary ν is that ν should contain wff's for every concept in the initial informal natural language description of the problem, e.g., for both ordering and permutation in the case of array sorting.

We give an algorithm for checking adequacy of ν and correcting an inadequate ν in Section V. This process of approximating the coarsest adequate vocabulary can be viewed as an *abstract interpretation* [8] problem.

Within this section, we assume that ν is adequate. Hence each $[V_\nu]$ is wholly contained in either vtt or in vff. Hence the union of all V_ν that are contained in vtt is exactly vtt: $vtt = (\bigcup V_\nu : [V_\nu] \subseteq vtt : [V_\nu])$. We can thus improve our tentative solution to $\mathcal{F} = (\bigvee V_\nu : [V_\nu] \subseteq vtt : fm(V_\nu))$. With a coarse enough ν, this will generate a succinct $\mathcal{F}$.

B. The formula construction algorithm

Our algorithm evaluates $\mathcal{F} = (\bigvee V_\nu : [V_\nu] \subseteq vtt : fm(V_\nu))$, i.e., it constructs $\mathcal{F}$ as the disjunction of the formulae $fm(V_\nu)$ for each V_ν contained in vtt. There are $2^{|\nu|}$ different assignments V_ν. We start with $\mathcal{F}$ set to false, and we loop through these. For each V_ν, we submit $fm(V_\nu)$ to a Satisfiability-modulo-theory (SMT) solver, e.g., Z3 [3]. An SMT solver takes as input a formula in a defined theory under first order logic. There are three possible outcomes: (1) the SMT solver exhausts its computational resources before determining if $fm(V_\nu)$ is satisfiable, (2) the SMT solver returns a satisfying assignment for $fm(V_\nu)$, and (3) the SMT solver returns that $fm(V_\nu)$ is unsatisfiable.

In case (1), our algorithm for constructing $\mathcal{F}$ terminates with failure. The developer can use the feedback from the failed attempt, such as the unsat core, to try to simplify the problem, e.g., by modifying ν, and then re-attempting. In case (2), a satisfying assignment σ is a partial assignment to the variables in $fm(V_\nu)$; i.e., a partial assignment to the variables in $vars(\nu)$. The remaining variables in $vars(\nu)$ can be assigned arbitrarily without affecting the satisfiability of $fm(V_\nu)$. Since we now have a value for each variable in $vars(\nu)$, we can interpret σ (augmented with the arbitrary assignments) as an element of Σ. We present σ to the developer, who determines whether $\sigma \in vtt$ or $\sigma \in vff$. Thus we really require the developer to classify an assignment σ as either "in the set of assignments for which the formula should be true" or "in the set of assignments for which the formula should be false", and we assume that this classification is accurate. If the developer responds "in vtt", then we conclude, by (Ad), that $[V_\nu] \subseteq vtt$. Hence we update $\mathcal{F}$ by disjoining $fm(V_\nu)$ to it, as indicated by the pseudocode line $\mathcal{F} := \mathcal{F} \frown \text{"}\vee\text{"} \frown fm(V_\nu)$ in Figure 1, where $\frown$ denotes string concatenation, i.e., we are constructing the text of the formula $\mathcal{F}$ as a concatenation of disjuncts. By construction, each disjunct $fm(V_\nu)$ is a conjunction of literals. Thus, $\mathcal{F}$ can be simplified each time a disjunct is added, using sum of products simplification, or all at once after ConstructFormula terminates. In case (3), we conclude, by (Ad), that $[V_\nu] \subseteq vff$, so we do not alter $\mathcal{F}$.

We iterate the above for every valuation $V_\nu : \nu \rightarrow \{tt, ff\}$ and so we compute $\mathcal{F}$ as the disjunction of the $fm(V_\nu)$ such that σ is in vtt. We annotate the pseudocode in Figure 1 with a loop invariant and some Hoare-style annotations. We use an auxiliary variable φ, which records the valuations V_ν that have been processed so far. The correctness of these annotations is self-evident from the pseudocode and the assumption of an adequate vocabulary ν. Figure 1 presents algorithm

$\mathsf{ConstructFormula}(\nu, vtt, vff)$ which takes as input a partition $\{vtt, vff\}$ of Σ and an adequate vocabulary ν, and returns a formula $\mathcal{F}$ such that $[\mathcal{F}] = vtt$. Theorem 1 below follows immediately from the previous discussion.

Theorem 1 (Correctness of ConstructFormula*):* Assume that (1) voc is *adequate* for (vtt, vff) and (2) that no invocation of the SMT solver by ConstructFormula fails, and (3) the developer responds accurately to all queries. Then ConstructFormula returns formula $\mathcal{F}$ such that $[\mathcal{F}] = vtt$.

C. Decidability and Complexity

ConstructFormula may fail to generate a formula if the SMT solver fails on any call. We are therefore interested in subclasses of first order logic where success is guaranteed. For example, when each of the $fm(V_\nu)$ formulae belongs to a class of formulae solvable in a finite domain, such as equality, monadic, and quantifier free theories [1], and array theories with one quantifier alternation under syntactic restrictions [4], [12] that can be reduced to the combined theory of equality with uninterpreted functions (EUF). Such theories are enough to express specifications such as sortedness and injectivity.

The running time of ConstructFormula is at most $2^{|\nu|}$ calls to the SMT solver, since everything else is straight-line code. Following are three improvements that in practice give us significant reductions in the number of calls to the solver.

We discuss next optimizations that further reduce the number of user queries needed.

1) Unsat-core elimination: When $fm(V_\nu)$ is found to be unsatisfiable, we obtain the unsat core from the SMT solver, and eliminate from consideration all V_ν that are extensions of the unsat core, since all of these will be unsatisfiable.

2) Partial-assignment elimination: The user can eliminate many valuations in one step as follows. When the user deems a presented assignment to be in vff, the user can select a subset of the variables assigned as the real reason for the choice. The partial assignment selected by the user may leave some of the subformulas in ν not evaluated to a truth value. For example, consider $\nu = \{C_1, C_2, C_3\}$ and consider a vff assignment $l = -1, r = 1$ where the user selects $l = -1$ as the reason for the vff decision. The partial assignment selected by the user evaluates C_1 and C_2 to a truth value, but leaves C_3 dependent on r. We learn that the valuation corresponding to $\neg C_1 \wedge \neg C_2 \wedge \neg C_3$ is also a vff without further querying the SMT solver and the user. We use the partial assignment selection by the user to reduce the number of valuations that we consider. We can apply this idea to vtt also, i.e., partial-assignment inclusion.

3) Hierarchical construction of vocabularies: We expect $|\nu|$ to be small in many cases, as it is the number of formulae used to construct a formula at the next level. In practice, we can keep the running time reasonable by constructing the vocabulary hierarchically, and structuring the levels of the hierarchy so that a formula is not constructed out of too many lower-level components. Such a long formula is difficult to write correctly using informal techniques, and so the methodological practices that make our method efficient are those that are a good idea in any case.

V. Adequacy of the vocabulary

We wish to verify that ν is adequate: $\Sigma/\nu \leqslant \{vtt, vff\}$. Proposition 2 gives us $\Sigma/\varepsilon \leqslant \Sigma/\nu$. Hence each $[V_\nu]$ is a union of some $[V_\varepsilon]$. Axiom-E gives us $\Sigma/\varepsilon \leqslant \{vtt, vff\}$, that is all the elements of each equivalence class $[V_\varepsilon]$ are in the same partition (vtt or vff) of Σ, and so it suffices to check a single representative of each $[V_\varepsilon]$. We check that the $[V_\varepsilon]$ that make up $[V_\nu]$ are either all contained in vtt, or all contained in vff. This implies that $[V_\nu]$ is contained in vtt or is contained in vff, i.e., $\Sigma/\nu \leqslant \{vtt, vff\}$.

We present an algorithm to check adequacy when ε and ν are both finite. We discuss in the next section how to handle general ε and ν. The check is implemented as follows. We iterate over all the $[V_\varepsilon]$, and for each we find a representative $\sigma_{V_\varepsilon} \in [V_\varepsilon]$ by invoking an SMT solver on $fm(V_\varepsilon)$. If $fm(V_\varepsilon)$ is not satisfiable, then it defines an empty partition of Σ/ε (which is certainly possible) and so we do nothing. Otherwise, a satisfying assignment gives a $\sigma_{V_\varepsilon} \in [V_\varepsilon]$. We query the user as to whether σ_{V_ε} is in vtt or in vff, and record the result.

We then iterate over all the V_ν, and for each we iterate over all the $[V_\varepsilon]$, checking if $\sigma_{V_\varepsilon} \models fm(V_\nu)$. If so, then $[V_\varepsilon] \subseteq [V_\nu]$ by the above discussion, since either all elements of $[V_\varepsilon]$ are in $[V_\nu]$ (and so satisfy $fm(V_\nu)$), or none are (in which case none satisfy $fm(V_\nu)$). We look up the classification of σ_{V_ε} (in vtt or in vff). If $\sigma_{V_\varepsilon} \in vtt$ then we know that V_ν intersects vtt, since $[V_\varepsilon] \subseteq [V_\nu]$. Likewise if $\sigma_{V_\varepsilon} \in vff$ then we know that V_ν intersects vff. A V_ν that intersects both vtt and vff is a cause of inadequacy of ν, since it causes $\Sigma/\nu \leqslant \{vtt, vff\}$ to be violated. We correct this by adding the "correction formula" $(\bigvee V_\varepsilon : \sigma_{V_\varepsilon} \models fm(V_\nu) \wedge side[V_\varepsilon] = \text{“}vtt\text{”} : fm(V_\varepsilon))$ to ν. This splits $[V_\nu]$ into $[V_\nu] \cap vtt$ and $[V_\nu] \cap vff$. We compute all such needed correction formulae and store them in an array $cfor[]$ which our algorithm, given in Figure 2, returns.

It follows from the above discussion that when all the correction formulae given by $cfor[]$ are added to ν, the result is an adequate vocabulary.

Theorem 2 (Correctness of MakeAdequate*):* Let $\mathsf{MakeAdequate}(\nu, \varepsilon, vtt, vff)$ return the array $cfor[]$ of correction formulae. Then $\nu \cup (\cup V_\nu \in \nu \mapsto \{tt, ff\} : cfor[V_\nu])$ is an adequate vocabulary.

VI. Finiteness and Decidability Considerations

We will discuss the the results of [4], namely a decidable fragment of first order logic that can express some properties of arrays in Section VII-A. Here we present our reduction of ε to ε_b, a finite version of ε where arrays have size b.

The algorithms given above assume that ε and ν are finite sets of wff's, since otherwise the number of equivalence classes is uncountable, in general. To remove this restriction, we first formalize the notation in which we express an equivalence theory. An element of Σ defines values for some scalar variables $\bar{z}$ (e.g., booleans and integers) and some arrays $\bar{a}$. For ease of exposition, we assume that there is exactly one array a. It is straightforward to remove this restriction. Let $\bar{i}$ be a set of "dummy" variables, which we use to index a.

```
ConstructFormula(ν, vtt, vff)
{Precondition: (vtt,vff) partitions Σ and Σ/ν ⩽ {vtt, vff} }
F := false; φ := V_ν ↦ {tt, ff}
{Invariant : F ≡ (⋁ V_ν : V_ν ∉ φ ∧ [V_ν] ⊆ vtt : fm(V_ν))}
while φ ≠ ∅
    select some valuation V_ν ∈ φ;
    φ := φ − V_ν;
    submit fm(V_ν) to an SMT solver;
    if the solver succeeds then
        if fm(V_ν) is satisfiable then
            let σ_v be the returned satisfying assignment;
            query the developer: is σ_v in vtt or in vff?
            if developer answers σ_v ∈ vtt then
                F := F ⌢ "∨" ⌢ fm(V_ν);          //can simplify F to improve succinctness
            else
                skip;          //can use partial assignment to reduce φ (Section IV-C2).
            endif
        else          //solver returned unsat
            let unsat ⊆ V_ν ↦ {tt, ff} be the unsat core valuations;
            φ := φ − unsat;          //unsat core reduction (Section IV-C1)
        endif
    else return("failure")          //return with failure since solver cannot answer query
    endif
endwhile
{Postcondition: F ≡ (⋁ V_ν : [V_ν] ⊆ vtt : fm(V_ν))}
return(F)
```

Fig. 1. ConstructFormula(ν, vtt, vff)

Definition 3 (Equivalence Theory Syntax): An equivalence theory ε consists of a finite number of *scalar formulae* $g_1(\bar{z}, |a|), \ldots, g_m(\bar{z}, |a|)$, and a finite number of *indexed formula set expressions* $\{f_1(\bar{z}, a, \bar{i}) \mid r_1(|a|, \bar{i})\}, \ldots, \{f_n(\bar{z}, a, \bar{i}) \mid r_n(|a|, \bar{i})\}$.

The range predicate $r(|a|, \bar{i})$ must be monotonic in $|a|$: for $b' > b$, $\{\bar{v} \mid r(\bar{v}, b)\} \subseteq \{\bar{v} \mid r(\bar{v}, b')\}$.
As indicated, a scalar formula can refer to the scalar variables $\bar{z}$ and to the size $|a|$ of array a. An indexed formula $f(\bar{z}, a, \bar{i})$ can refer to the $\bar{z}$, and to elements of a by using any of $\bar{i}$ as an index. The range predicate $r(|a|, \bar{i})$ can refer to $\bar{i}$ and $|a|$.

Definition 4 (Bounded Equivalence Theory ε_b): For $b > 0$ and equivalence theory ε, the equivalence theory with bound b, ε_b, is the set of wffs $\{g_1(\bar{z}, b), \ldots, g_m(\bar{z}, b)\} \cup \{f_1(\bar{z}, a, \bar{i}) \mid r_1(b, \bar{i})\}, \cup \ldots \cup, \{f_n(\bar{z}, a, \bar{i}) \mid r_n(b, \bar{i})\}$. Each formula set expression $\{f(\bar{z}, a, \bar{i}) \mid r(b, \bar{i})\}$ denotes the set of formulae consisting of $f(\bar{z}, a, \bar{v})$ for each $\bar{v}$ such that $r(b, \bar{v})$. Example: search of an array a between indices ℓ and r inclusive:

- $\ell = r$, $\ell < r$
- $\ell \geqslant 0$, $\ell \leqslant |a| - 1$,
  $\{\ell = c$ for all c such that $0 \leqslant c < |a|\}$
- $r \geqslant 0$, $r \leqslant |a| - 1$,
  $\{r = c$ for all c such that $0 \leqslant c < |a|\}$
- $\{a[i] = e$ for all i such that $0 \leqslant i < |a|\}$

For $|a| = 5$, we obtain:

- $\ell = r$, $\ell < r$
- $\ell \geqslant 0$, $\ell \leqslant 4$, $\ell = 0$, $\ell = 1$, $\ell = 2$, $\ell = 3$, $\ell = 4$
- $r \geqslant 0$, $r \leqslant 4$, $r = 0$, $r = 1$, $r = 2$, $r = 3$, $r = 4$
- $a[0] = e$, $a[1] = e$, $a[2] = e$, $a[3] = e$, $a[4] = e$

Here c and i are the dummies.

We wish to find a "threshold" β such that we can execute our algorithms using ε_β instead of ε. Since ε is the union of ε_b for all $b > 0$, we must show how every ε_b can be "represented" in ε_β. We require that every satisfiable valuation V_{ε_b} in ε_b have a representative valuation in ε_β. We will then process this representative, rather than V_{ε_b}. If we can do this for all valuations V_{ε_b} for all $b > \beta$, then we can replace reasoning about the infinite theory ε with reasoning about the finite theory ε_β.

Given β, b such that $\beta < b$, we define the mapping $M_{\beta b} : \varepsilon_\beta \mapsto \varepsilon_b$ as follows. For $j = 1, \ldots, m$, $g_j(\bar{z}, \beta)$ maps to $g_j(\bar{z}, b)$. For $k = 1, \ldots, m$, $f_k(\bar{z}, a, \bar{v})$ maps to $f_k(\bar{z}, a, \bar{v})$ for each $\bar{v}$ such that $r_k(\beta, \bar{v})$ holds. Note that $r_k(b, \bar{v})$ also holds, by monotonicity of range predicates.

For each valuation V_{ε_b}, we define the projection onto ε_β, $V_{\varepsilon_b} \upharpoonright \varepsilon_\beta$: for every $f \in \varepsilon_\beta$, $V_{\varepsilon_b} \upharpoonright \varepsilon_\beta(f) = V_{\varepsilon_b}(M_{\beta b}(f))$. That is, we evaluate a formula f of ε_β in $V_{\varepsilon_b} \upharpoonright \varepsilon_\beta$ by mapping it to V_{ε_b} using $M_{\beta b}$, and then applying V_{ε_b}.

```
MakeAdequate(ν, ε, vtt, vff)

{Precondition: ν and ε are finite}
foreach valuation V_ε : ε → {tt, ff}
    submit fm(V_ε) to an SMT solver;
    if the solver cannot answer the query
        terminate with failure;
    else if the solver succeeds and returns that fm(V_ε) is not satisfiable then;
        skip;
    else
        let σ_{V_ε} ⊨ fm(V_ε) be satisfying assignment returned by solver;        //σ ∈ [V_ε]
        query the developer: is σ in vtt or in vff?
        side[V_ε] := answer of developer        //either "vtt" or "vff". Store in side[V_ε]
endfor

foreach valuation V_ν : ν → {tt, ff}
    foreach valuation V_ε : ε → {tt, ff}
        if σ_{V_ε} ⊨ fm(V_ν)        //[V_ε] ⊆ [V_ν]
            sides[V_ν] := sides[V_ν] ∪ side[V_ε]        //V_ν intersects side[V_ε]
    endfor        //Accumulate in sides[V_ν]

endfor

foreach valuation V_ν : ν → {tt, ff}
    if sides[Vv] = {vtt, vff}        //V_ν intersects vtt and vff
        cfor[V_ν] := (⋁ V_ε : σ_{V_ε} ⊨ fm(V_ν) ∧ side[V_ε] = vtt : fm(V_ε))
    else
        cfor[V_ν] := true
    endif
endfor
return(cfor[]);
```

Fig. 2. MakeAdequate$(\nu, \varepsilon, vtt, vf\!f)$

We will use $V_{\varepsilon_b} \upharpoonright \varepsilon_\beta$ as the representative of V_{ε_b}. For our algorithms to work correctly under this mapping, we require, for some β and all $b > \beta$:

1) If V_{ε_b} is satisfiable, then so is $V_{\varepsilon_b} \upharpoonright \varepsilon_\beta$. That is, if $[V_{\varepsilon_b}] \neq \emptyset$, then $[V_{\varepsilon_b} \upharpoonright \varepsilon_\beta] \neq \emptyset$.
2) For all $\sigma_b \in [V_{\varepsilon_b}]$, $\sigma_\beta \in [V_{\varepsilon_b} \upharpoonright \varepsilon_\beta]$, the user classifies σ_b and σ_β in the same way, i.e., both in vtt or both in $vf\!f$.

Clause 1 can be checked mechanically by submitting it to a SMT solver. Our first attempt to write Clause 1 as a first order wff is:

$$\exists\, \beta \forall\, b > \beta : (\exists\!\!| fm(V_{\varepsilon_b})) \ \Rightarrow \ (\exists\!\!| fm(V_{\varepsilon_b} \upharpoonright \varepsilon_\beta)),$$

where we render each occurrence of $\exists\!\!|$ using existential quantification over boolean variables, i.e., bits.

However, the formulae in ε_b depend on b, which presents a problem: $(\exists\!\!| fm(V_{\varepsilon_b}))$ is a wff which depends on b, so that different b give different formulae. Thus, we have to check an infinite set of wff's, one for each b. We deal with this by verifying a single formula which implies each of these wff's.

Define $fm(V_{\varepsilon_b}) \triangleq fm(V^s_{\varepsilon_b}) \wedge fm(V^i_{\varepsilon_b})$, where $fm(V^s_{\varepsilon_b})$ is the assignment to the scalar formulae in ε_b, and $fm(V^i_{\varepsilon_b})$ is the assignment to the indexed formulae in ε_b. Likewise define $fm(V_{\varepsilon_\beta}) \triangleq fm(V^s_{\varepsilon_\beta}) \wedge fm(V^i_{\varepsilon_\beta})$, where $V_{\varepsilon_\beta} \triangleq V_{\varepsilon_b} \upharpoonright \varepsilon_\beta$. We wish to check

$$(\exists\!\!| fm(V^s_{\varepsilon_b}) \wedge fm(V^i_{\varepsilon_b})) \Rightarrow (\exists\!\!| fm(V^s_{\varepsilon_\beta}) \wedge fm(V^i_{\varepsilon_\beta})).$$

By monotonicity of range predicates, we have $\varepsilon^i_\beta \subseteq \varepsilon^i_b$, where $\varepsilon^i_\beta, \varepsilon^i_b$ are the subsets of $\varepsilon_\beta, \varepsilon_b$ respectively, consisting of the indexed formulae. Hence $fm(V^i_{\varepsilon_b}) \Rightarrow fm(V^i_{\varepsilon_\beta})$ is logically valid. So

$$(\exists\!\!| fm(V^s_{\varepsilon_b}) \wedge fm(V^i_{\varepsilon_b})) \ \Rightarrow \ (\exists\!\!| fm(V^s_{\varepsilon_b}) \wedge fm(V^i_{\varepsilon_\beta}))$$

is also logically valid. Hence it suffices to check

$$(\exists\!\!| fm(V^s_{\varepsilon_b}) \wedge fm(V^i_{\varepsilon_\beta})) \ \Rightarrow \ (\exists\!\!| fm(V^s_{\varepsilon_\beta}) \wedge fm(V^i_{\varepsilon_\beta})).$$

Since the set of scalar formulae is fixed (does not vary with b), the above depends only on β. We therefore render it as a wff as follows:

$$\forall\, b > 0 : (\exists\, \bar{z}, a : fm(V^s_{\varepsilon_b}) \wedge fm(V^i_{\varepsilon_\beta})) \Rightarrow (\exists\, \bar{z}, a : fm(V^s_{\varepsilon_\beta}) \wedge fm(V^i_{\varepsilon_\beta})). \qquad \text{Th}(\beta)$$

This is still not quite a wff, since it is not closed: it depends on β. We cannot add a $\exists\, \beta$ quantifier at the beginning, since the form of the formula changes with β (same problem we had above with b). So, we check Th(β) for values of β starting from 1 and incrementing. Hence, we find the smallest value of β which works, as desired.

Clause 2 must be assumed as an axiom, since it is a restriction on user behavior:

User-Consistency: Let $b > \beta$, and let $V_{\varepsilon_\beta} = V_{\varepsilon_b} \upharpoonright \varepsilon_\beta$. Then the user assigns the same classification (*vtt* or *vff*) to all $\sigma_b \in [V_{\varepsilon_b}]$, and $\sigma_\beta \in [V_{\varepsilon_b} \upharpoonright \varepsilon_\beta]$.

From Clauses 1 and 2, we obtain:

for all $b \geqslant \beta$, if some $\sigma \in [V_{\varepsilon_b}]$ exists, then some $\sigma_\beta \in [V_{\varepsilon_\beta}]$ exists, and the user gives the same answers to the queries $\sigma \in vtt$ and $\sigma_\beta \in vtt$.

Hence we can present $\sigma_\beta \in vtt$? to the developer rather than $\sigma \in vtt$?

a) Example: array search.: Let ε be the equivalence theory for array search given above. Then for ε_b, the scalar formulae are $\ell = r$, $\ell < r$, $\ell < r - 1$, $\ell \geqslant 0$, $\ell \leqslant b - 1$, $r \geqslant 0$, $r \leqslant b - 1$, and the indexed formulae are $\ell = 0, \ell = 1, \dots \ell = b - 1$, $r = 0, r = 1, \dots, r = b - 1$, $a[0] = e, a[1] = e, \dots, a[b-1] = e$.

Now for ε_β with $\beta < b$, the scalar formulae are $\ell = r$, $\ell < r$, $\ell < r - 1$, $\ell \geqslant 0$, $\ell \leqslant \beta - 1$, $r \geqslant 0$, $r \leqslant \beta - 1$, and the indexed formulae are $\ell = 0, \ell = 1, \dots \ell = \beta - 1$, $r = 0, r = 1, \dots, r = \beta - 1$, $a[0] = e, a[1] = e, \dots, a[\beta - 1] = e$.

Note that the indexed formulae of ε_β are a subset of those of ε_b, while the scalar formula are not: they result by substituting β for b.

Let V_{ε_b} be an assignment to $\ell = r$, $\ell < r$, $\ell \geqslant 0$, $\ell \leqslant b - 1$, $r \geqslant 0$, $r \leqslant b - 1$, $\ell = 0, \ell = 1, \dots \ell = \beta - 1$, $r = 0, r = 1, \dots, r = \beta - 1$, $a[0] = e, a[1] = e, \dots, a[\beta - 1] = e$.

Let V_{ε_β} be an assignment to $\ell = r$, $\ell < r$, $\ell \geqslant 0$, $\ell \leqslant \beta - 1$, $r \geqslant 0$, $r \leqslant \beta - 1$, $\ell = 0, \ell = 1, \dots \ell = \beta - 1$, $r = 0, r = 1, \dots, r = \beta - 1$, $a[0] = e, a[1] = e, \dots, a[\beta - 1] = e$.

Th(β) states that if V_{ε_b} is satisfiable, then so is V_{ε_β}. Suppose that V_{ε_b} assigns true to $\ell < r$, $\ell \geqslant 0$, $r \leqslant b - 1$, and truth values to other formulae so that V_{ε_b} is satisfiable. Then V_{ε_β} assigns true to $\ell < r$, $\ell \geqslant 0$, $r \leqslant \beta - 1$, and must also be satisfiable. This requires $\beta \geqslant 2$. If we had included $\ell < r - 1$ in ε, e.g., to require at least one array element between the left and right boundaries, then we would have $\beta \geqslant 3$. We validated this by composing Th(β) manually and submitting to Z3, with values 1,2,3 for β. Th(β) was not valid for 1,2, and was valid for 3, as expected.

These lower bounds on β show that we need ε_β to have array sizes sufficiently large to be able to represent all satisfiable assignments to the formulae in any ε_b.

VII. Vocabulary and Quantifier Construction

We present our vocabulary construction method, and then present three complementary methods to construct quantified formulae. Our vocabulary construction method takes as input:

- A type theory τ expressed as a set of, variables X and a map from X to scalar and array types,
- A set of literal constants L such as $0, 1, true$, and $false$,
- A Presburger and index operations alphabet $\Sigma = \{index, bound, =, <=, +, -, *, []\}$,
- A grammar $G \subseteq X \times X \cup L \times 2^\Sigma$, denoting the allowed operations between variables,
- A bound K expressing the maximum number of allowed operations in a clause

The method then traverses the grammar G and builds ν to be the set of all Boolean formulae with up to K operators. We pass ν to ConstructFormula. This relieves the user from providing both ν and ε since we can also use an extended grammar G' and a larger bound $K' > K$ for ε.

A. Quantified formula construction

The work in [12] and [4] discuss decidable fragments of the theories of sequences and arrays. The *array property theory* $\exists\forall_i\tau$ presented in [4] allows restricted existential and universal quantification of the form $\forall \bar{x}.\phi(\bar{x}) \rightarrow \psi(\bar{x})$. $\exists\forall_i\tau$ limits universal quantification to the variables used in index terms, limits Presburger arithmetic expressions used in ϕ for quantified variables, and allows Presburger arithmetic and Boolean operations in ϕ and ψ. $\exists\forall_i\tau$ is defined by a grammar which restricts the syntax of formulae appropriately.

Satisfiability of $\exists\forall_i\tau$ is polynomially reducible to satisfiability of quantifier free, uninterpreted functions, equality theory (QF-EUF) with additional free variables each of which replaces one universally quantified variable [4].

The quantified formula construction method takes an additional bound N from the user denoting the maximum number of quantified variables. The method constructs the set $X' = X \cup X_N$ where X_N has up to N fresh scalar variables, and constructs the set G' by adding rules to G that relate the fresh variables in X_N to the array variables in X. The method then traverses the grammar G' and builds $\exists\forall_i^N\tau^K$ the set of all Boolean formulae with up to K operators. The construction of the $\exists\forall_i^N\tau^K$ theory is further detailed online[1].

If the grammar provided by the user is within the grammar of [4] and [12], then the theory $\exists\forall_i^N\tau^K$ is a subset of $\exists\forall_i\tau$; it is reducible to QF-EUF which renders queries to the SMT solver decidable. $\exists\forall_i^N\tau^K$ is also powerful enough to express formulae under the array property and the list property theories with up to N quantifiers and K-operation Boolean terms. We leave the grammar restriction as a user choice to benefit from other decidable theories covered by the SMT solvers.

We use $\exists\forall_i^N\tau^K$ as our vocabulary and we run ConstructFormula to construct the desired formula. When querying the user, we hide the values of the X_N variables. In practice, if a presented assignment is not enough to judge vtt or vff, this is an indication that the generated vocab is not adequate and that the user should increase either N or K.

Once ConstructFormula returns $\mathcal{F}$, we deskolmnize it and construct $\exists\bar{X_N}.\mathcal{F}_{k-1}$ by existentially quantifying the X_N variables in $\mathcal{F}$ that were not part of the original type theory provided by the user. This works well, since $\mathcal{F}$ is a disjunction of vocabulary evaluations (each of which is a conjunction of clauses) and existential quantification distributes through disjunction. This allows us to move the $\exists$ to the beginning of $\mathcal{F}$, as in $\exists\bar{X_N}.\mathcal{F}_{k-1}$.

For example, the method took the `Input` type theory and grammar in Figure 3 that specified an array a, two bounds ℓ and r, and a scalar e denoted of element sort by the `(a,e,=)` grammar rule, extended the variable set with i, added the rule `(a,i,index)` to the grammar, generated a vocab with $K = 1$ and called ConstructFormula to construct the formula `eina(a,left,right,e)` specifying that e is in a between ℓ and r inclusive.

The method also took the type theory that specified a as an array, and one grammar rule `(a,a,<=)` rule that allowed elements of a to be compared with each other, injected the variable i as an index to a, constructed a vocab that with $k = 3$ that included a Presburger index term $i + 1$, called ConstructFormula to generate the formula `notsorted(a)`. The formula `notsorted(a)` can be negated to express `sorted(a)`. The generated formulae can then be used as vocabulary clauses in the construction of other formulae.

Note that, the same method can be applied to obtain universally quantified formulae with a variant of ConstructFormula where we construct $\neg\mathcal{F}$, the complement of $\mathcal{F}$, where we start with *true* instead of *false*, and proceed to trim the formula $\neg\mathcal{F}$ by conjunctions of formulae corresponding to vocab evaluations deemed *vff* by the user; instead of adding disjunctions of those deemed *vtt* to $\mathcal{F}$. Therefore, a `sorted(a)` can be generated directly as a universally quantified formula.

B. Hierarchical and Incremental Construction

Our method builds the formula in incremental steps from bottom to top. Let $\mathcal{F}_{k-1}$ be a formula generated at level $k-1$. We deskolemize it and generate $\exists\bar{x}.\mathcal{F}_{k-1}$ where $\bar{x}$ represents the variables in $\mathcal{F}_{k-1}$ that are not part of τ_k, the type theory of $\mathcal{F}_k$. We then introduce $\exists\bar{x}.\mathcal{F}_{k-1}$ as a clause C in the vocabulary of $\mathcal{F}_k$.

Consider the formula `eina(a,left,right,e)` from Figure 3 constructed to express the existence of element e in array a between bounds ℓ (`left`) and r (`right`) in the process of constructing $\mathcal{F}$; a postcondition for linear search. We deskolemnize and introduce `eina(a,left,right,e)`$=\exists i.\mathcal{F}_{k-1}$ as a clause C in the construction of $\mathcal{F}$. We use C along with other vocabulary clauses, resulting in $(0 \leqslant \ell \leqslant r \leqslant |a| - 1) \wedge \big((rv \neq -1 \wedge e = a[rv] \wedge eina(a, \ell, r, e)) \vee (rv = -1 \wedge \neg eina(a, \ell, r, e))\big)$ where the negation introduces a universal quantifier. Figure 3 shows a sample output for the linear search postcondition using the incremental method.

We could have written the linear search postcondition directly without using the `eina` clause. However, that results in more queries to the user and the SMT solver. Building formulae incrementally also builds a rich library of accurate reusable specifications.

VIII. Implementation

The implementation of ConstructFormula and MakeAdequate is available online [1]. The tool `sc` implements ConstructFormula and takes a type theory τ as a set of variable declarations. It also takes a vocabulary ν as a set of SMT formulae. Optionally, it takes a grammar that relates the variables to each other, and generates a vocabulary ν_g from the type theory and the grammar. The user has the option to produce a quantifier free equivalent of the ν or ν_g if they are under the array or the list property theories [4], [12] to guarantee successful SMT calls.

[1] http://webfea.fea.aub.edu.lb/fadi/dkwk/doku.php?id=speccheck

```
eina(a,left,right,e)

Input: theory eina {
  int [] a; int left; int right; int e;
  grammar { (a,left,bound); (a,right,bound); (a,e,=);} }
...
Spec: exists i. 0<= left and left <= right
        and right <= a.size - 1
        and left <= i and i <= right and a[i]=e
```

```
not-sorted(a)

Input: theory not-sorted {
  int [] a;
  grammar { (a,a,<=);}}
...
Spec: exists i. 0 <= i and i <= a.size - 1 and
            0 <= i + 1 and i + 1 <= a.size - 1  and
            not (a[i] <= a[i+1])
```

```
array-search-post(a,left,right,e,rv)

input: theory ls-post {
  int [] a; int left; int right; int e; int rv;
    bool eina(a,left,right,e);
  grammar { (a,left,bound); (a,right,bound);
    (a,rv,index); (a,e,=);} }
...
Spec: 0 <= left and left <= right and right <= a.size - 1
      and (rv = -1  and !eina(a,left,right,e) or
           rv != -1 and eina(a,left,right,e) and a[rv]=e)
```

Fig. 3. Sample formulae generated using ConstructFormula

The user also specifies other options such as the maximum number of quantifiers, the type of the quantifier, and the maximum number of operations per generated vocabulary clause. Upon successful termination, the tool uses ESPRESSO [5] and ABC [24], logic synthesis tools, to simplify the specification. The simplified specification is then presented to the user.

The tool `ma` takes a type theory τ, an equivalence theory ε, and a vocabulary ν and augments ν if needed so that it is adequate as described in MakeAdequate. All tools use the C++ api of the Z3 SMT solver [3].

IX. Results

We conducted a user experiment using the array search and the array sorted examples. Table I shows the results. Eight volunteer students and two logic design experts were asked to construct specifications using `sc`. They were trained to use `sc` with simple examples that specify orders between scalars. Then they were given `sc` with an assignment sheet that instructed to specify the following.

- `eina(a,left,right,e)` using a startup vocab.
- `eina(a,left,right,e)` using a type theory and a grammar.
- Incrementally specifying the array search property.
- sorted(a).

TABLE I

RESULTS OF USER EXPERIMENTS WITH SC

Spec	User	Attempts	Clauses	Accuracy	User Queries	SMT Queries	Used PA	SMT time 10^{-6}(seconds)	Total time (s)
eina, user vocab: 3 clauses, inject quantifier	student	3	5	correct	8	14	0	4190	821
		1	3	missed range on i	8	8	2	3299	715
		1	3	missed range on i	5	5	3	2302	748.09
		2	5	correct	8	10	1	2991	542.213
		1	3	correct	8	8	0	2667	76
	expert	1	5	correct	8	10	1	2785	543
		1	5	correct	8	10	1	2855	588
eina , type theory , generated	student	2	20	correct	125	182	7	57558	2329
		3	20	correct	243	323	4	113870	1934.72
		1	20	correct	84	153	7	43232	1468.87
		2	20	correct	59	117	9	30699	1584.01
		2	20	correct	31	69	11	12194	746.3
	expert	1	20	correct	44	88	9	20785	1096
		1	20	correct	33	71	10	13042	770
linear search, type theory, incremental	student	2	20	correct	30	79	6	19296	717
		3	20	correct	243	323	4	113870	1934.72
		1	5	missed-rv=-1	25	29	1	10355	230.488
		1	5	correct	10	11	3	3500	496.174
		1	5	correct	32	32	0	3138	336.851
		1	5	missed-rv=-1	9	10	3	3970	256.58
		2	20	correct	37	91	5	15321	362.972
	expert	1	20	correct	28	72	7	12241	543
sorted, type theory	student	1	7	correct	19	23	2	7529	406
		1	7	missed-i+1 bound	36	40	1	13032	234.696
		2	7	correct	26	30	2	10178	221.476
		2	7	correct	36	40	0	13232	181.09
		2	7	correct	11	15	5	3506	270
	expert	1	7	correct	12	12	4	5598	420

The tool currently has no undo facility, so users aborted the run when they provided an unintentional (mistaken) answer. They were not allowed to attempt again once they achieved a constructed specification. The attempts column reflects the number of aborted attempts by the user, plus the final attempt.

We explained the partial assignment optimizations to the users, and we warned them against using them. They still used them to save time, especially with the generated vocabulary. Users who specified partial assignments made mistakes more often and forced the tool to ignore valid vtt assignments. Some users, who used the optimizations to save time, ended up calling the SMT solver less often, but spent more total time discerning their optimizations. All users, including the two experts, reported their surprise on how much easier it was to construct the `sorted` property compared to the `search` property using the tool. The accuracy of the constructed formulae was jointly assessed by the users and the authors. Some users left early, due to timing constraints.

The authors of the tool also validated the tool by writing accurate specifications for memory allocation and deallocation, linked list validity, binary search tree properties, red black binary search tree properties, rooted index tree properties, and a text justify example. The assignment sheet and samples from the logged results are available online[1].

X. RELATED WORK

The methods in [16], [15], [17], [21], [7] work by writing the specification and then attempting to verify if it is accurate using animation, execution, model-checking, etc. We go in the other direction: we write the specification from the behaviors, so that the specification is accurate by construction. A method of writing temporal-logic based specifications using event traces ("scenarios") is presented in [25]. It applies to reactive systems and stresses control rather than data. In [11], a method for refining an initially simple specification using informal "elaborations" is presented. A method of checking software cost reduction (SCR) specifications for consistency is presented in [18]. Zeller in [26] discusses writing specifications as models discovered from existing software artifacts of relevance to the desired functionality. In none of the above is there an analogue to our construction of preconditions and postconditions as formulae of first order logic.

In [20], an oracle-based method computes a loop free program that requires a distinguishing constraint and an I/O behavior constraint. The method either synthesizes a program or claims the provided components are insufficient. We differ in that we build specifications in first order logic with quantifiers, we do not require the "correctness" of ε, and we correct ν when it is not adequate.

The SPECIFIER [23] tool constructs formal specifications of data types and programs from informal descriptions, but uses schemas, analogy, and difference-based reasoning, rather than input-output behaviors. Larch [13] enables the verification of claims about specifications, which improves the confidence in the specification's accuracy. In [22], a method for testing preconditions, postconditions, and state invariants, using mutation analysis, is presented.

XI. CONCLUSION

We presented a method to construct a formal specification, given (1) an adequate formal vocabulary, and (2) interaction with a user who can accurately classify behaviors. We illustrated our method with examples and evaluated it by conducting user experiments. We illustrated our method by constructing specifications for array search, binary search, red black binary search trees, and root indexed trees. We also conducted a controlled experiment with senior undergraduate and graduate students and logic design experts.

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