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Verified Model Checking for Conjunctive Positive Logic

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Abstract We formalize, in the Dafny language and verifier, a proof system PS for deciding the model checking problem of the fragment of first-order logic, denoted $\mathcal{FO}(\forall, \exists, \land)$, known as Conjunctive Positive Logic (CPL). We mechanize the proofs of soundness and completeness of PS ensuring its correctness. Our formalization is representative of how various popular verification systems can be used to verify the correctness of rule-based formal systems on the basis of the least fixpoint semantics. Further, exploiting Dafny automatic code generation, from completenes proof we achieve a mechanically verified prototype implementation of a proof search mechanism that is a model checker for CPL. The model checking problem of $\mathcal{FO}(\forall, \exists, \land)$ is equivalent to the quantified constraint satisfaction problem (QCSP), and it is PSPACE-complete. The formalized proof system provides a way of detecting tractability cases for the general QCSP and it can be applied to arbitrary formulae of CPL.

Keywords Conjunctive Positive Logic · Quantified Constraint Satisfaction Problem · Proof System · Model Checking · Verification · Dafny.

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1 Introduction

Model checking [14,40] is the problem of deciding whether a logical sentence holds for a structure or not. It is a fundamental computational task that appears in areas such as computational logic, verification, artificial intelligence, constraint satisfaction, and computational complexity. The case where the logical sentence is a first-order sentence and the structure is finite is of interest mainly in database theory. In general, model checking problem is intractable. To be precise, model checking for first-order logic is PSPACE-complete [46]. All in all, model checking for fragments of first-order logic appears as an important challenge.

The (quantified) conjunctive positive fragment of first-order logic, in symbols $\mathcal{FO}(\forall, \exists, \land)$, contains all first-order sentences built on atoms using only logical symbols in $\{\forall, \exists, \land\}$, where an atom is the application of a predicate $R(x_1, \ldots, x_n)$ where x_1, \ldots, x_n are variable symbols (in a fixed countable set) and R is a relation (or predicate) symbol. This fragment is commonly called *Conjunctive Positive Logic* (*CPL*). The fragment $\mathcal{FO}(\exists, \land)$ is called *Existential Conjunctive Positive Logic* and its model checking problem is equivalent to the much-studied *Constraint Satisfaction Problem* (*CSP*), whereas the model checking problem of $\mathcal{FO}(\forall, \exists, \land)$ is equivalent to the *Quantified Constraint Satisfaction Problem* (*QCSP*)[35].

CSP provides a general framework in which a wide variety of combinatorial search problems can be expressed in a natural way [17,18]. An instance of the CSP can be viewed as a collection of predicates over a set of variables. The aim is to determine whether there exist values for all of the variables such that all of the specified predicates hold simultaneously. Henceforth, from a logic approach, the CSP is viewed as the model checking problem for $\mathcal{FO}(\exists, \land)$. This approach has proven to be very successful due to the connection between the logic notion of definability and the complexity of the CSP [11]. The CSP is NP-hard (actually, it is NP-complete). Indeed, in [12] a 3SAT instance is expressed by a CSP instance where all variables range over a boolean domain and predicates correspond to the clauses (thus the arity of each predicate is 3). Although the CSP is NP-complete in general, there are additional restrictions on the input instances that make the problem easier. One of the main aims of research in CSP is to identify and classify tractable special cases of the general problem. The theoretical literature on CSP mainly investigates two kind of restrictions. The first type is to restrict the type of predicates that are allowed. This direction includes the classical work of Schaefer [43] and its many generalizations. The second type is to restrict the structure induced by the predicates on the variables [25, 38]. QCSP is a natural generalization of the CSP and it can be viewed as the model checking problem for Conjunctive Positive Logic (or $\mathcal{FO}(\forall, \exists, \land))$). A study of complexity of the model checking problem of various fragments of first-order logic can be found in [36], whereas a good, and quite recent, survey on the QCSP and close problems is [37]. QCSP is actively studied in artificial intelligence, where it is used to model problems, for example, in non-monotonic reasoning [19] and in planning [42]. Various general (superpolynomial or incomplete) algorithms for the QCSP over the boolean domain have been suggested [9, 10, 24, 50], and quite recently researchers have started investigations on solving non-boolean QCSP problems [7,23,34,50]. Since QBF can be expressed as a QCSP instance [12], the general QCSP is PSPACE-complete. Like in the CSP case, a lot of research is being done nowadays trying to find tractable instances.It is in this context where a proof system for QCSP, called PS, was introduced in [1].

This proof system provides a way of detecting tractability cases for the general QCSP. PS is a slight variant of the proof system previously defined in [13]. The study of the proofs that can be generated by PS is a good tool to discover lower bounds in proof complexity, and even on the running time of algorithms that determine the satisfiability of formulas. A good understanding of how PS proofs are generated provides clues on the very nature of PSPACE-complete problems [13]. So far, the main motivation to formalize PS. Besides, the restriction of PS to the boolean domain turns out PS into a proof system that simulates Q-resolution [13], which many of the so-called QBF-solvers are based on. Q-resolution was introduced in [9]. After, many different extensions and variants has been proposed, such as Long-Distance resolution [3, 52], QU-resolution [22], and LQU-resolution [4] which combines Long-Distance and universal resolution. It is worth noting that all these systems are defined in the propositional setting whereas PS works over any finite domain. This is a strength of PS because some scenarios are more naturally and cleanly modelled by allowing variables to be quantified over domains of size greater than two.

Automated reasoners have turned out to be useful tools in a wide range of areas from pure mathematics to smart contracts. Automated reasoners play a vital role in formalizing and certifying computation related engines, such as compilers, virtual machines, operating systems, protocols, programming languages, solvers, checkers, etc. Very often, formalizations are very long and complicated, and certificate proofs are error-prone and difficult to check by hand. Henceforth, there is genuine value in having mechanized (machine-checked) proofs. Interactive theorem provers or proof assistants, such as Agda [8], Coq [49] and Isabelle/HOL [39], have been successfully used for this task for many years, producing an extensive collection of system formalizations and mechanized proofs. An excellent extensive review on proof-assistants developments of different kinds of software systems is [41]. Machine-checked formalizations of logical systems [51] and checkers (or solvers) [5, [20, 44, 45] are quite recent. In [20, 45] executable code is generated from the verified formalization of the system. Automatic program verifiers – such as ACL2 [27], VCC [16], F* [47], VeriFast [26], Why [21] and Dafny [28]- are dedicated reasoners to verify behavioral properties of programs written in some specific programming language. It has been recently shown [15] that program verifiers environments are also suitable for formalization of rule-based systems. Consequently, the program verification 'style' has joined the challenge of formalizing logical systems and automatically generating the code of verified checkers or solvers. Proving metaproperties of proof systems -such as soundness, completeness, and many others related to proof search-makes heavy use of advanced logic constructs, thus typically involves complex reasoning steps, beyond first-order logic. Program verifiers has extended their specification language (beyond first-order logic) with, among other, constructions that allow to reason about fixpoints in an automated way. Fixpoint reasoning is crucial to encode rule-based systems (hence, logical systems) and to prove meta-logical properties of the inference system, respectively. The reason for that is that well-founded (or terminating) recursive functions and predicates (i.e. whose recursive calls are made on arguments that are structurally smaller) are, in general, not expressive enough to represent the set of all the statements that can be proved using a set of rules. In other words, the least derivability relation induced by the a set of inference rules cannot be defined using well-founded recursion. Proof assistants provide, since long, support for fixpoint reasoning, typically

with user-interaction. More recently a mostly-automatic kind of fixpoint reasoning has been introduced in program verification tools. In [6] the authors explain some examples using fixpoint formalizations in Why3. In [15] the first formalization of a rule-based system, using mostly-automatic fixpoint reasoning, is introduced. In [33] fixpoint reasoning for Dafny was introduced, providing a novel support for automatically proving lemmas using fixpoint induction. Consequently, Dafny provides a strong support to formalize logical systems, to verify its soundness and completeness (and other interesting properties), and also to generate code for their corresponding provers, checker or solvers. In addition, a significant challenge to construct large mechanized proofs is the ability to control the logical context of the proved properties, in two senses. On one hand, for clarity and easy human reading, well-defined dependencies between definitions and properties are really helpful. On the other hand, the performance of automated provers is improved as the set of logical premises needed to prove a lemma is well delimited. Dafny also provides a module system that allows the user to split formalizations into small components and to make explicit scopes and dependencies. Another Dafny feature we exploit in this work is automatic code generation that allows to generate .NET code for any verified program. To the best of our knowledge, there is no published work that substantiates all these Dafny features by presenting a (modular) formalization of a dedicated formal system and the prover-style tool obtained by automatic code generation.

In this paper we present a Dafny formalization of the proof system [1], called PS, the machine-checked proofs of its soundness and completeness, and the model checker obtained by automatic code generation. Along the presentation, we expose the constructors used inside Dafny to encode the system and to prove the main lemmas. We emphasize the fixpoint reasoning from, both, the theoretical view applied to PS and its practical use in proving the soundness of PS. We also report on our experience doing this work. The MVS-project can be downloaded from site http://github.com/alexlesaka/VMC_CPL, and the verified model checker is available as a web application at http://qcspmc.ikerlan.es.

Outline of the paper. In Section 2 we introduce the proof system PS and its least fixpoint operator. In Section 3 we provide basic notions of the Dafny language and verifier. In Section 4 we describe the formalization of the proof system PS as an inductive predicate with all the technical details. In Section 5, we explain the main ideas behind the mechanized proofs of soundness and completeness. In Section 6 we explain the structure of modules and its dependencies of our formalization, whereas in Sections 7 and 8 we respectively give implementation and experience details.

2 A Proof System for QCSP

In this section we introduce the proof system PS, along with all the necessary basic notions on QCSP, taken from [1,13]. We also relate PS with the least fixpoint of the derivability relation.

We focus on the sublogic of relational first-order logic known as Conjunctive Positive Logic (CPL). A signature σ is a finite set of relation symbols; each relation symbol $R \in \sigma$ has an associated arity $\operatorname{ar}(R)$ which is an element of \mathbb{N} . An atom is an application of a predicate $R(x_1 \dots x_{\mathsf{ar}(R)})$, where $x_1 \dots x_{\mathsf{ar}(R)}$ are variable symbols (in a fixed countable set) or constant symbols, and $R \in \sigma$. A formula (over signature σ) is built from atoms (over σ), conjunction (\wedge), universal quantification (\forall), and existential quantification (\exists). A *sentence* is a formula having no free variables.

A structure **B** on signature σ consists of a domain *B* of **B**, which is a finite non-empty set and, for each symbol $R \in \sigma$, a relation $R^{\mathbf{B}} \subseteq B^{\operatorname{ar}(R)}$. We call an *interpretation* to the map that associates to each symbol *R* a relation $B^{\operatorname{ar}(R)}$. For a structure **B** and a sentence ϕ over the same signature, we write $\mathbf{B} \models \phi$ if the sentence ϕ is true in the structure **B**.

A QCSP instance is a pair (ϕ, \mathbf{B}) where ϕ is a sentence in CPL, and **B** is a structure, such that all the relation symbols in ϕ belong to the signature of **B**. The QCSP is the problem of deciding, given a QCSP instance (ϕ, \mathbf{B}) , whether or not $\mathbf{B} \models \phi$.

Example 1 We show that 3-QBF –the case of the QBF problem where every clause has exactly three literals– can be expressed as a QCSP. Define the relations $R_{0,3}, R_{1,3}, R_{2,3}$, and $R_{0,3}$ by

$$\begin{array}{l} R_{0,3} = \{0,1\}^3 \setminus \{(0,0,0)\}, \\ R_{1,3} = \{0,1\}^3 \setminus \{(1,0,0)\}, \\ R_{2,3} = \{0,1\}^3 \setminus \{(1,1,0)\}, \\ R_{3,3} = \{0,1\}^3 \setminus \{(1,1,1)\}, \end{array}$$

Then, for any variables x, y, z, we have the following equivalences:

$$R_{0,3}(x, y, z) = (x \lor y \lor z),$$

$$R_{1,3}(x, y, z) = (\neg x \lor y \lor z),$$

$$R_{2,3}(x, y, z) = (\neg x \lor \neg y \lor z),$$

$$R_{3,3}(x, y, z) = (\neg x \lor \neg y \lor \neg z),$$

in the sense that, for example, the constraint $R_{1,3}(x, y, z)$ is satisfied by an assignment if and only if the clause $(\neg x \lor y \lor z)$ is satisfied by the assignment. In general, let σ be the signature $\{R_{0,3}, R_{1,3}, R_{2,3}, R_{3,3}\}$ and **B** the structure with domain = $\{0, 1\}$ and such that $R_{0,3}^{\mathbf{B}}, R_{1,3}^{\mathbf{B}}, R_{2,3}^{\mathbf{B}}$, and $R_{3,3}^{\mathbf{B}}$ are defined as above. Every instance of the 3-QBF problem can be readily translated into an instance of QCSP having the same satisfying assignments. For example, the 3-QBF instance

$$\forall s \exists t \,\forall u \,\exists v \,((\neg u \lor s \lor \neg t) \land (\neg s \lor t \lor v) \land (s \lor t \lor \neg v) \land (v \lor u \lor s)).$$

is equivalent to the QCSP instance (φ, \mathbf{B}) where

$$\varphi = \forall s \exists t \forall u \exists v (R_{2,3}(u,t,s) \land R_{1,3}(s,t,v) \land R_{1,3}(v,s,t) \land R_{3,3}(v,u,s)).$$

For our purposes, formulas are seen as trees. The proof system enables to derive what we call *constraints* at the various nodes of the tree. To facilitate the discussion, we will assume that each sentence ϕ has, associated with it, a set I_{ϕ} of *indices* that contains one index for each subformula occurrence of ϕ , that is, for each node of the tree corresponding for ϕ . In other words, we use an indexing, by a set I_{ϕ} , of the tree that represents a formula ϕ . Let us remark that (in general) the collection of constraints derivable at an occurrence of a subformula does not depend only on the subformula and on the structure, but also on the subformula's

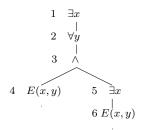


Fig. 1 Formula discussed in Example 2 (from [13]).

location in the full formula ϕ . When *i* is an index, we use $\phi(i)$ to denote the actual subformula of the formula occurrence corresponding to *i*; we will also refer to *i* as a *location*.

Example 2 Consider the sentence $\phi = \exists x \forall y (E(x, y) \land (\exists x E(x, y)))$ (see Figure 1). When viewed as a tree, this formula has 6 nodes. We can index the representation of ϕ as a tree, according to the depth-first search order, by the index set $\{1, \dots, 6\}$. Then, we have that $\phi(6) = E(x, y), \phi(5) = \exists x \phi(6), \phi(4) = E(x, y), \phi(3) = \phi(4) \land \phi(5), \phi(2) = \forall y \phi(3), \text{ and } \phi(1) = \exists x \phi(2).$

We say that an index i is a *parent* of an index j, and also that j is a *child* of i, if, in viewing the formula ϕ as a tree, the root of the subformula occurrence of i is the parent of the root of the subformula occurrence of j. Note that, when this holds, the formula $\phi(i)$ either is of the form $Qv\phi(j)$ where Q is a quantifier and v is a variable, or is a conjunction where $\phi(j)$ appears as a conjunct. For example, with respect to the sentence and indexing in Example 2, index 3 has two children whose index are 4 and 5, and index 3 has one parent whose index is 2.

Definition 1 (Judgement) Let (ϕ, \mathbf{B}) be a QCSP instance. A *constraint* on (ϕ, \mathbf{B}) is a pair (V, F) where V is a set of variables occurring in ϕ , and F is a set of mappings from V to B. A *judgement* on (ϕ, \mathbf{B}) is a triple (i, V, F) where $i \in I_{\phi}$ and (V, F) is a constraint with $V \subseteq \mathsf{freeVar}(\phi(i))$; it is *empty* if $F = \emptyset$.

Roughly speaking, the role of a judgement (i, V, F) on (ϕ, \mathbf{B}) is to collect in F the mappings f on the variables V that are "candidates" to satisfy $\mathbf{B}, f \models \phi(i)$. The construction of judgements is based on operations over mappings (from variables to elements of the domain) and sets of mappings. When \mathbf{B} is a structure, ϕ is a formula over the vocabulary of \mathbf{B} and f is a mapping from the free variables of ϕ to the universe of \mathbf{B} , we write $\mathbf{B}, f \models \phi$ to indicate that ϕ is satisfied in \mathbf{B} under f. When f is a mapping and $z \in B$, we use $f[x \mapsto v]$ to denote the extension or update of f that maps x to v. This notation is also used multiple updating as $f[x_1 \mapsto v_1, \ldots, x_n \mapsto v_n]$ and also $f[X \mapsto V]$ where X, V respectively represents the tuples $(x_1 \ldots, x_n)$ and $(v_1 \ldots, v_n)$. When f is mapping from V to B and U is a subset of V, we use $f \upharpoonright U$ to denote the restriction of f to U.

Definition 2 (Operations over sets of mappings) Let (U_1, F_1) , (U_2, F_2) be two constraints on the same QCSP instance, we define the *join* of F_1 and F_2 , denoted by $F_1 \bowtie F_2$, to be

$$F_1 \bowtie F_2 = \{ f : U_1 \cup U_2 \to B \mid (f \upharpoonright U_1) \in F_1, (f \upharpoonright U_2) \in F_2 \}$$

Let (V, F) be a constraint and $U \subseteq V$ with $\{w_1, w_2, \ldots, w_r\} = V \setminus U$, we define the *projection* and the *dual-projection* of F on U, respectively denoted by $F \upharpoonright U$ and F # U, to be

$$F \upharpoonright U = \{ f \upharpoonright U : U \to B \mid f \in F \}$$
$$F \# U = \{ f : U \to B \mid f[w_1 \mapsto b_1, \dots, w_r \mapsto b_r] \in F \text{ for all } b_1, b_2, \dots, b_r \in B \}.$$

The dual-projection is used to deal with universally quantified variables. Dually, projection can be used to cope with existential quantification. We adopt the convention that (relative to a QCSP instance) there is exactly one map $e : \emptyset \to B$ defined on the empty set, so there are two constraints whose variable set is the empty set: the constraint (\emptyset, \emptyset) , and the constraint $(\emptyset, \{e\})$ where e is the aforementioned map.

The proof system PS is refutation-based in the sense that it aims to find a proof of the empty judgement $(-, \emptyset, \emptyset)$ on (ϕ, \mathbf{B}) , which means that $\mathbf{B} \not\models \phi$. The next definition introduces the inference rules of the proof system PS, as it was defined in [1].

Definition 3 (*PS* **proof system**) A judgement proof on a QCSP-instance (ϕ , **B**) on signature σ is a finite sequence of judgements, each of which is obtained by the application of the following inference rules:

(atom)
$$\overline{(i, V, F)}$$
 where
$$\begin{cases} R \in \sigma \text{ such that } \operatorname{ar}(R) = k \\ V = \{v_1, \cdots, v_k\} \\ \phi(i) = R(V) \\ F = \{f : V \to B \mid (f(v_1), ..., f(v_k)) \in R^{\mathbf{B}} \} \end{cases}$$

(join)
$$\frac{(i, U_1, F_1) \quad (i, U_2, F_2)}{(i, U_1 \cup U_2, F_1 \bowtie F_2)}$$

(projection)
$$\frac{(i, V, F)}{(i, U, F \upharpoonright U)}$$
 where $U \subseteq V$

$$(\forall \text{-elimination}) \ \frac{(j, V, F)}{(i, V \setminus \{y\}, F \# (V \setminus \{y\}))} \text{ where } \begin{cases} y \in V \\ \phi(i) = \forall y \phi(j) \\ i \text{ is the parent of } j \end{cases}$$

(upward flow) $\frac{(j, V, F)}{(i, V, F)}$ where *i* is the parent of *j*

Given an instance (ϕ, \mathbf{B}) , we say that a judgement (i, V, F) is *derivable* on (ϕ, \mathbf{B}) if there exists a judgement proof on (ϕ, \mathbf{B}) that contains (i, V, F).

It is worthy noting that Definition 1 requires of a triple (i, V, F), to be a judgement, that all variables in V must be free variables of $\phi(i)$. Consequently, since PS only deals with judgements, the (upward flow) rule can only be applied to a judgement (j, V, F) if all variables in V are free variables of $\phi(i)$, where i is the parent of j.

In Example (3) we present a judgement proof according to PS, where $(1, \emptyset, \emptyset)$ is derived. It also shows how the combination of both the upward flow rule and the projection rule derives judgements where the number of variables is minimum.

Obviously, the correctness of the upward flow rule relies in the fact that CPL logical symbols $(\forall, \exists, \land)$ are 'positive'.

Example 3 Let ϕ be the sentence from Example 2 over signature $\sigma = \{E\}$ with ar(E) = 2. Consider ϕ to be indexed as shown in Figure 1, where $\phi(6) = E(x, y)$, $\phi(5) = \exists x \phi(6), \phi(4) = E(x, y), \phi(3) = \phi(4) \land \phi(5), \phi(2) = \forall y \phi(3), \text{ and } \phi(1) = \exists x \phi(2)$. Let **B** be the structure over σ with domain $B = \{a, b, c\}$ such that $E^{\mathbf{B}} = \{(a, a), (a, c), (b, a)\}$. Let G_E be the set of mappings from $\{x, y\}$ to B that satisfy E(x, y) (over **B**):

$$G_E = \{\{x \mapsto a, y \mapsto a\}, \{x \mapsto a, y \mapsto c\}, \{x \mapsto b, y \mapsto a\}\}$$

A possible judgement proof on (ϕ, \mathbf{B}) is the following.

 $\begin{array}{ll} (1)-\ ({\rm atom}): & (6,\{x,y\},G_E) \\ (2)-\ {\rm From}\ (1)\ {\rm by}\ ({\rm projection}): & (6,\{y\},\{\{y\mapsto a\},\{y\mapsto c\}\}) \\ (3)-\ {\rm From}\ (2)\ {\rm by}\ ({\rm upward}\ {\rm flow}): & (5,\{y\},\{\{y\mapsto a\},\{y\mapsto c\}\}) \\ (4)-\ {\rm From}\ (3)\ {\rm by}\ ({\rm upward}\ {\rm flow}): & (3,\{y\},\{\{y\mapsto a\},\{y\mapsto c\}\}) \\ (5)-\ {\rm From}\ (4)\ {\rm by}\ (\forall\mbox{-elimination}):\ (2,\emptyset,\emptyset) \\ (6)-\ {\rm From}\ (5)\ {\rm by}\ ({\rm upward}\ {\rm flow}):\ (1,\emptyset,\emptyset) \\ \end{array}$

The work presented in this paper is based on viewing the set of statements that can be derived by a proof system as the least fixpoint of the derivability relation that is induced by the set of inference rules of the considered proof system. Next, we illustrate this view of the proof system PS to provide a good basis of the general theory underlying our formalization.

The set of all judgements that are derivable on a given QCSP instance (ϕ, \mathbf{B}) can be seen as a least fixpoint of an operator that we call $D_{(\phi,\mathbf{B})}$. Next, we formally define this operator. Let \mathcal{J} be the set of all derived judgements on a QCSP instance (ϕ, \mathbf{B}) . The set $\mathcal{P}(\mathcal{J})$ (all subsets over \mathcal{J}) is a partial ordered defined by the \subseteq -relation among sets. $D_{(\phi,\mathbf{B})}$ is a map from $\mathcal{P}(\mathcal{J})$ to $\mathcal{P}(\mathcal{J})$ which, given any $S \in \mathcal{P}(\mathcal{J})$, is defined as

 $D_{(\phi,\mathbf{B})}(S) = S \cup \{ j \in \mathcal{J} \mid j \text{ is obtained by applying one of the inference}$ rules to a judgement $s \in S \}.$

Given any QCSP instance (ϕ, \mathbf{B}) , the least fixpoint of $D_{(\phi, \mathbf{B})}$ is the set of all derivable judgementes according to the fixpoint semantics.

Example 4 Let ϕ be the sentence $\phi = \exists x \forall y P(x, y)$ where $\phi(3) = P(x, y)$; $\phi(2) = \forall y \phi(3)$; $\phi(1) = \exists x \phi(2)$. Consider ϕ as a sentence over signature $\{P\}$ with ar(P) = 2. Define **B** to be a structure over this signature having domain $B = \{a, b, c\}$ and where $P^{\mathbf{B}} = \{(a, a), (a, b)\}$

Let F_P be the set of mappings from $\{x, y\}$ to B that satisfy P(x, y) (over **B**):

$$F_P = \{ \{ x \mapsto a, y \mapsto a \}, \{ x \mapsto a, y \mapsto b \} \}.$$

For this QCSP instance we calculate the fixpoint of $D_{(\phi,\mathbf{B})}$.

Therefore, the empty judgement $(1, \emptyset, \emptyset)$ belongs to the least fixpoint of the derivability relation associated to the studied QCSP-instance.

Example 5 Let ϕ be the sentence from Example 2 over signature $\sigma = \{E\}$ with ar(E) = 2. Consider ϕ to be indexed as shown in Figure 1, where $\phi(6) = E(x, y)$, $\phi(5) = \exists x \phi(6), \phi(4) = E(x, y), \phi(3) = \phi(4) \land \phi(5), \phi(2) = \forall y \phi(3), \text{ and } \phi(1) = \exists x \phi(2)$. Let **B** be the structure over σ with domain $B = \{a, b, c\}$ such that $E^{\mathbf{B}} = \{(a, a), (a, b), (a, c), (b, a)\}$. Let F_E be the set of mappings from $\{x, y\}$ to B that satisfy E(x, y) (over **B**):

$$F_E = \{ \{x \mapsto a, y \mapsto a\}, \{x \mapsto a, y \mapsto b\}, \{x \mapsto a, y \mapsto c\}, \{x \mapsto b, y \mapsto a\} \}.$$

The least fixpoint of $D_{(\phi,\mathbf{B})}$ is calculated below, where K is the set of mappings $\{\{x \mapsto a\}, \{x \mapsto b\}\}.$

$$\begin{split} D_{(\phi,\mathbf{B})} \uparrow 0 &= \emptyset \\ D_{(\phi,\mathbf{B})} \uparrow 1 &= \{(4, \{x, y\}, F_E), (6, \{x, y\}, F_E)\} \\ D_{(\phi,\mathbf{B})} \uparrow 2 &= D_{(\phi,\mathbf{B})} \uparrow 1 \cup \{(4, \{y\}, H), (4, \emptyset, \{e\}), (4, \{x\}, K), \\ &\qquad (6, \{y\}, H), (6, \emptyset, \{e\}), (6, \{x\}, K), (3, \{x, y\}, F_E)\} \\ D_{(\phi,\mathbf{B})} \uparrow 3 &= D_{(\phi,\mathbf{B})} \uparrow 2 \cup \{(3, \{y\}, H), (3, \emptyset, \{e\}), (3, \{x\}, K), \\ &\qquad (5, \{y\}, H), (5, \emptyset, \{e\}), (2, \{x\}, G)\} \\ D_{(\phi,\mathbf{B})} \uparrow 4 &= D_{(\phi,\mathbf{B})} \uparrow 3 \cup \{(2, \emptyset, \{e\}), (2, \{x\}, K)\} \\ D_{(\phi,\mathbf{B})} \uparrow 5 &= D_{(\phi,\mathbf{B})} \uparrow 4 \cup \{(1, \emptyset, \{e\})\} \\ D_{(\phi,\mathbf{B})} \uparrow 6 &= D_{(\phi,\mathbf{B})} \uparrow 5 \text{ which is the least fixpoint.} \end{split}$$

Hence, the empty judgement $(1, \emptyset, \emptyset)$ is not in the fixpoint of $D_{(\phi, \mathbf{B})}$. This means that the empty judgement cannot appear in any judgement proof on the considered QCSP-instance.

It is obvious, by construction, that the least fixpoint of $D_{(\phi,\mathbf{B})}$ is the set of all judgements that are derivable on (ϕ, \mathbf{B}) . Consequently, metalogical properties of the set of all judgements that are derivable on (ϕ, \mathbf{B}) can be proved by induction on the number of iterations of the operator $D_{(\phi,\mathbf{B})}$. By Tarski's Theorem [48], the existence of the least fixpoint of the operator $D_{(\phi,\mathbf{B})}$ (over the boolean lattice) requires $D_{(\phi,\mathbf{B})}$ to be monotonic, hence such fact should be also ensured to validate any inductive proof on the number of iterations.

The next theorem establishes the correctness and completeness of PS. Its proof has been made in Dafny on the basis of the least fixpoint semantics, and it is one of the main contribution of this work.

Theorem 1 (Correctness and Completeness of *PS*) Let (ϕ, \mathbf{B}) be a QCSP instance. Assume the root of ϕ has index r. The empty judgement $(r, \emptyset, \emptyset)$ is derivable if and only if $\mathbf{B} \not\models \phi$.

In Example 4, the empty judgement $(1, \emptyset, \emptyset)$ is derivable. Therefore, by Theorem 1, $\mathbf{B} \not\models \phi$. In Example 5, the empty judgement $(1, \emptyset, \emptyset)$ is not in the least fixpoint of $D_{(\phi, \mathbf{B})}$, by Theorem 1, it holds that $\mathbf{B} \models \phi$.

3 Dafny: Language, Verifier and IDE

Dafny [28] is a program verifier that includes a programming language and specification constructs. The Dafny user creates and verifies both specifications and implementations. Dafny specification language extends first-order logic with algebraic data types, extreme/inductive predicates, induction (also co-induction), generic types, abstracting and refining modules, assertions and many others builtin specification features that makes Dafny a good candidate for our work. In this section, we briefly introduce the main notions of Dafny that facilitates the understanding of the rest of the paper.

The basic unit of a Dafny program is the method. A method is a piece of executable code with a head where multiple named parameters and multiple named results are declared. Dafny has also built-in specification constructs for assertions, such as requires for preconditions, ensures for postconditions, and assert for inline assertions. Using requires and ensures we specify methods and lemmas. Assertions specify properties that are satisfied at some point. Assertions are mainly used to provide hints to the verifier. In other words, once the assertion is proved, it turns into a usable property for completing the proof. Indeed, "assert φ " tells Dafny to check that φ holds and to use the condition φ (as a lemma) to prove the properties beyond this point. Dafny distinguishes between *ghost* entities and executable entities. Ghost entities are used only during verification; the compiler omits them from the executable code. The lemma declarations are like methods, but no code is generated for them, i.e. a lemma is equivalent to ghost method. The body of a lemma is its proof. Dafny also offers user-defined specification constructs (which are ghost), such as function and predicate that can be defined by well-founded inductive definitions, built-in immutable types, polymorphic (inductive and coinductive) algebraic datatypes, inductive and co-inductive predicates. Dafny also provides built-in immutable type, such as set, multiset, map and seq -which respectively denote the types of finite sets, multisets, maps, tuples, and sequences- that are very useful in specification. These built-in types are equipped with the usual operations, including set comprehension expressions:

set x1 : T1, x2:T2, ... | P(x1,x2,...) • E(x1,x2,...)

for defining the set of all values given by the expression E(x1,x2,...) for all finite tuples (x1,x2,...) such that P(x1,x2,...).¹ For lemma proofs, Dafny provides a special notation that is easy to read and understand: *calculations* [30]. A calculation in Dafny is a statement that proves a property. This notation was extracted from the *calculational method* [2], whereby a theorem is established by a chain of formulas, each transformed in some way into the next. The relationship between successive formulas (for example, equality, implication, double implication, etc.) is notated, or it can be omitted if it is the default relationship (equality). In addition, the hints (usually asserts or lemma calls) that justify a step can also be notated (in curly brackets after the relationship). Calculations are written inside the environment calc{ }.

The Dafny specification constructor inductive predicate (also called *extreme* predicates) [33] allows the definition of a predicate as an extreme solution: a least fixpoint of a set of recursive rules.² Inductive predicates are essential to formally define the set of judgments that can be proved by the proof system PS (introduced in the previous section). Properties of inductive predicates can be proved by induction in the construction of the least fixpoint of an inductive predicate P(x). Such properties must be coded as inductive lemmas for least fixpoint. Dafny offers a standard way to set up the proof of these kind of lemmas, by induction on the number of iterations of the operator whose least fixpoint is the meaning of P(x). To validate such inductive proofs, according to Tarski's Theorem [48], Dafny verifies the monotonicity of P, by checking out that every call to P (in its definition) is under an even number of negations. Very detailed and helpful explanations on inductive predicates and inductive lemmas can be found in [33]. In Section 4 we introduce an inductive predicate (is_derivable) and prove an inductive lemma (models_Lemma).

The Dafny integrated development environment (IDE) is an extension of Microsoft Visual Studio (VS). The IDE is designed to reduce the effort required by the user to make use of the system. The IDE runs the program verifier in the background and provides design time feedback. Assertions are sent to the SMT solver Z3 (a fully automatic theorem prover) to check its satisfiability that will be reported to the Dafny user. Assertion violations in lemma proofs, as well as verification errors, are reported along with different informations such as the locations (of the properties) related to the error. The interested reader is referred to [31] for further information on the several ways that Dafny IDE helps to build both lemma proofs and verified software. Dafny is able to export executable files (.exe), libraries (.dll) and .Net source code (.cs) with the implementation of the functionality specified, whenever the automatic verification is successful and every lemma is proved.

¹ For easy reading, in the Dafny code snippets, we show the usual mathematical symbols, instead of real Dafny notation. For example, we show • for ::(such that), \cup for union instead of +, \subseteq for set inclusion instead of <=, also for the logical symbols and quantifiers, for example && is shown as \land and forall as \forall , etc.

 $^{^2\,}$ Dafny also provides co-induction based on greatest fixpoints (see [33]), but they are not used in this paper.

4 Formalization of the Proof System PS in Dafny

In this section we explain the main types and definitions that make up our formalization. We first formalize what are (well-formed) structures, formulas, QCSP-Instances and judgements. Then, we define the operations on judgements and the inductive predicate that formalizes the derivability relation of PS.

Structures A structure is given by a triple formed by a signature, a domain (i.e. a non-empty finite set), and an interpretation, which is a map from the names in the signature to relations on the domain of the arity determined in the signature.

```
type Name = string
type Signature = map<Name,int>
type Interpret<T> = map<Name,set<seq<T>>>
datatype Structure<T> =
        Structure(Sig: Signature,Dom: set<T>,I: Interpret<T>)
predicate wfStructure<T>(B: Structure<T>)
{
B.Dom ≠ {} ^
∀ r • r in B.Sig.Keys ⇒ (r in B.I ^
        ∀ t • t in B.I[r] ⇒ |t| = B.Sig[r])
}
```

The variable of type T represents the type of the elements in the domain, relations in the domain are represented by the set of sequences (viewed as tuples) that belongs to the relation. Hence, the predicate wfStructure decides the non-emptiness of the domain along with every relation symbol is interpreted by sequences whose length is its arity.

Formulas and QCSP-instances We define the syntax of Conjunctive Positive Logic formulas as a datatype, where for example an atom R(x1, x2, x3) is represented as Atom("R", [x1,x2,x3]). In the datatype Formula each constructor has two destructors giving access to each component of the formula.

```
datatype Formula =
                      Atom(rel:Name, par:seq<Name>)
                    | And(O:Formula, 1:Formula)
                    | Forall(x: Name, Body: Formula)
                    | Exists(x: Name, Body: Formula)
predicate wfFormula(S: Signature, phi: Formula)
match phi
   case Atom(R, par) => R in S.Keys \land |par| = S[R]
   case And(phi0, phi1) => wfFormula(S, phi0) ^ wfFormula(S, phi1)
   case Forall(x, alpha) => wfFormula(S,alpha)
   case Exists(x, alpha) => wfFormula(S,alpha)
7
function freeVar(phi:Formula): set<Name>
ſ
match phi
   case Atom(R, par) => setOf(par)
   case And(ph1, phi1) => freeVar(ph1) + freeVar(phi1)
```

```
case Forall(x, phi) => freeVar(phi) - {x}
case Exists(x, phi) => freeVar(phi) - {x}
}
predicate sentence(phi:Formula) { freeVar(phi) = {} }
```

The predicate wfFormula decides whether a formula is well-formed with respect to a given signature, that is if the number of parameters of all its atoms coincides with its arity. The function freeVar gives the set of its free variables, and the predicate sentence decides whether a formula has no free variables.

```
predicate wfQCSP_Instance(phi:Formula, B:Structure)
{
wfStructure(B) \lambda wfFormula(B.Sig,phi) \lambda sentence(phi)
}
```

A weel-formed QCSP-instance consist of a well-formed structure, a well-formed formula with symbols in the signature of the structure that must be a sentence. For example, if phi is Exists(x,Forall(y,And(Atom(E,[x, y]),Exists(x,Atom(E,[x,y])))))and B is $\texttt{Structure}(\texttt{map}[\texttt{E}\mapsto\texttt{2}],\texttt{set}\{a,b,c\},\texttt{map}[\texttt{E}\mapsto\texttt{set}\{[a,a],[a,b],[a,c],[b,a]\}])$ which represents the QCSP-intance of Example 3, then wfQCSP_Instance(phi, B) is True.

 $Judgements\,$ We also declare judgements and the predicate for checking its well-formedness as follows: 3

A (well-formed) judgement on a (well-formed) QCSP-instance (ϕ, \mathbf{B}) , as defined in Section 2, is a triple formed by an index i on the set of index of ϕ , a set of variables included in the free variables of the subformula of index i of ϕ and a set of maps from exactly these variables to elements of the domain of the structure. For that, setOfIndex is a function that computes the set of indexes in the nodes of a given formula (seen as a tree, see Figure 1). In our formalization, for easy access to formula nodes, indexes are sequences of zeros and ones, instead of natural numbers. We do not explain here the technical details of that formalization. Given an index i, a formula phi and a signature S, the function called FoI(i, phi, S) returns the subformula of phi of index i. The parameter s is added for expressing that the function FoI preserves the well-formedness property with respect to the signature of phi.

Operations on judgements The inference rules in PS rely upon apply the operations join, projection and dual-projection on the sets of valuations, which are

 $^{^3\,}$ In Dafny code, one line comments start by // and are coloured in green.

part of one or two judgements (the component F in the datatype) associated to a QCSP-instance given by a formula ϕ and a structure B. We define (in Dafny) the following predicates on judgements to decide whether a judgement is a projection or a dual-projection of another judgement, and also whether a judgement is the joint of two given judgements.

```
predicate is_projection<T> (j1: Judgement<T>, j2: Judgement<T>,
                         phi: Formula, B: Structure <T>)
// j1 is a projection of j2
Ł
predicate is_dualProjection<T> (j1: Judgement<T>, v: Name,
                             j2: Judgement <T>
                             phi:Formula, B:Structure<T>)
// j1 is a dual projection of j2 (on variable v)
j2.i = j1.i + [0] \land j1.V = j2.V - {v} \land v in j2.V \land
j1.F = (set h: Valuation <T> | h in allMaps(j1.V, B.Dom) \land
                          \forall b • b in B.Dom \implies h[v:=b] in j2.F)
7
predicate is_join<T> (j: Judgement<T>, j1: Judgement<T>,
                    j2: Judgement <T>, phi: Formula, B: Structure <T>)
// j is the join of j1 and j2
requires wfJudgement(j,phi,B)
ſ
\texttt{j.i} = \texttt{j1.i} = \texttt{j2.i} \land \texttt{j.V} = \texttt{j1.V} + \texttt{j2.V} \land
j.F = (set f: Valuation <T> | f in allMaps(j1.V+j2.V, B.Dom) \land
                         projectVal(f,j1.V) in j1.F ~\wedge
                         projectVal(f,j2.V) in j2.F)
}
```

For a judgement j, the expression j.i is the index in the tree that represents the formula, and j.i + [0] (respectively j.i + [1]) is the index of its left-hand (resp. right-hand) child. If it has only one child, it is j.i + [0]. Function projectVal, when applied to any f: Valuation<T> and any U: set<Name>) such that $U \subseteq f.Keys$, calculates (map s | s in U • f[s]): Valuation<T>, hence projectVal(f,U).Keys =U is ensured. In the above predicate is_join, Dafny checks the finiteness of the set allMaps(j1.V+j2.V, B.Dom). Indeed, Dafny checks the finiteness of X for any expression x in X where X is a set. Function allMaps gives the set of all maps whose domain is keys and whose range is a subset of values. Indeed, we prove this fact in lemma allMaps_Correct_Lemma.

The above three predicates is_join, is_projection and is_dualProjection, along with the following predicate is_upwardFlow respectively enable the encoding of the inference rule (join), (projection), (\forall -elimination) and (upward flow), which are given in Definition 3.

requires wfJudgement(j1,phi,B) ^ wfJudgement(j2,phi,B)
{
 j2.V = j1.V ^ j2.F = j1.F ^
 (
 (FoI(j1.i,phi,B.Sig).And? ^ (j2.i = j1.i+[0] ∨ j2.i = j1.i+[1]))
 ((FoI(j1.i,phi,B.Sig).Forall? ∨ FoI(j1.i,phi,B.Sig).Exists?) ^
 j2.i=j1.i+[0])
}

Derivability predicate The following inductive predicate is_derivable defines, in a very natural way, the least fixpoint of the derivability relation induced by the five rules in Definition 3.

```
inductive predicate is_derivable <T(!new)> (j: Judgement <T>,
                                        phi: Formula,
                                        B: Structure <T>)
Ł
var phii := FoI(j.i,phi,B.Sig);
( // rule (atom)
phii.Atom?
\land j.V = setOf(phii.par)
\land j.F = (set f: Valuation < T > | f in allMaps(j.V, B.Dom)
                            A HOmap(f,phii.par) in B.I[phii.rel])
) \vee ( // rule (projection)
∃ j' • wfJudgement(j',phi,B) ∧ is_projection(j,j',phi,B)
            ∧ is_derivable(j',phi,B)
) \vee ( // rule (join)
phii.And?
. ∃ j0,j1 •
           wfJudgement(j0,phi,B) \land wfJudgement(j1,phi,B)
            \wedge j0.i = j1.i
            ∧ is_join(j,j0,j1,phi,B)
            ) \vee ( // rule (\forall-elimination)
phii.Forall?
\land \exists j' \bullet wfJudgement(j', phi, B)
        ^ phii=Forall(phii.x,FoI(j'.i,phi,B.Sig))
        ^ is_dualProjection(j,phii.x,j',phi,B)
        ∧ is_derivable(j',phi,B)
) \vee ( // rule (upward flow)
∃j'

    wfJudgement(j',phi,B)

         ^ is_upwardFlow(j,j',phi,B) ^ is_derivable(j',phi,B)
)
}
```

In Dafny, inductive predicate definitions are not allowed to depend on the allocation state. The suffix (!new), on parameter type T (it is shown as superindex in the Dafny code snippets), restricts the instances of T to types that do not contain any reference to an object (or pointer), and thus does not depend on the allocation state. This is a quite recently added type-parameter characteristic (!new), in the same vein as the suffix (==) restricts instances to be equalitysupporting types.

In the encoding of the rule (atom), we use the auxiliary function HOmap for applying the function f to the list of arguments phii.par, this gives a tuple that is checked to belong to the interpretation of relation phii.R in the structure B.

5 Dafny Proofs of Soundness and Completeness

In this section we explain the main ingredients of the Dafny proof for Theorem 1, which ensures that PS is a sound and complete proof system for QCSP instances. The forward direction of Theorem 1 states the soundness result that is proved in Dafny lemma soundness_Theorem. The backward direction is the completeness statement that is proved by the Dafny lemma completeness_Theorem. For expressing these meta-logical results we use the following predicate that states whether a QCSP-instance (B,f) is a model of a formula phi.

The above three recursive cases are obvious. The case Atom(R,par), using the auxiliary function HOmap, applies the function f to the list of arguments par, and checks if the resulting tuple belongs to the interpretation of relation R in the structure B.

On the basis of the above predicate models, we define:

Given a valuation h and a judgement j on a QCSP-instance (phi,B), predicate valuationModel decides whether (B,h) models the subformula of phi given by the index of j.i properly closed with existential quantifiers on all the variables that do not belong to j.V. The expression FoI(j.i,phi,B.Sig)) represents the formula $\phi(i)$, the expression freeVar(FoI(j.i,phi,B.Sig))-j.V represents freeVar($\phi(i)$)\j.V and the function existSq enables the existential closing (for its definition see Figure 3 at the end of Section 6). Hence, the Dafny expression

existSq(freeVar(FoI(j.i,phi,B.Sig))-j.V,FoI(j.i,phi,B.Sig))

encodes the formula $\exists x_1 \dots \exists x_n \phi(i)$ provided that $\mathsf{freeVar}(\phi(i)) \setminus j. \forall = \{x_1, \dots, x_n\}$. The soundness_Theorem will be prove as an easy consequence of the following:

Lemma 1 Let (ϕ, \mathbf{B}) be a QCSP instance and (i, V, F) a derivable judgement (on *it*). Let $\{v_1, v_2, \ldots v_n\}$ be the variables in freeVar $(\phi(i)) \setminus V$. For all $h : V \to B$ it holds that $\mathbf{B}, h \models \exists v_1 \ldots \exists v_n \phi(i)$ implies $h \in F$.

which is encoded in Dafny as the following inductive lemma, whose proof is partially shown:

```
inductive lemma models_Lemma<T> (j: Judgement<T>, phi: Formula,
                            B: Structure <T>)
requires is_derivable(j,phi,B)
ensures \forall h • valuationModel(h,j,phi,B) \implies h in j.F
ſ
∧ j.F = (set f: Valuation <T> | f in allMaps(j.V,B.Dom)
                       A HOmap(f,phii.par) in B.I[phii.rel])
{// (atom)
\forall h | valuationModel(h,j,phi,B) {allMaps_Correct_Lemma(h,B.Dom);}
7
else if ∃ j' • wfJudgement(j',phi,B) ∧ is_projection(j,j',phi,B)
                                  ∧ is_derivable(j', phi, B)
{// (projection)
∧ is_derivable(j', phi, B);
models_Lemma(j',phi,B);
projection_Lemma(j,j',phi,B);
7
else if ... {// (join)
}
else if ... {// (\forall-elimination)
7
else {// (upward flow)
}
}
```

Since models_Lemma is an inductive lemma with hypothesis is_derivable(j,phi,B), the proof makes induction in the construction of the inductive predicate is_derivable, the inductive proof of models_Lemma has a base case for the rule (atom) and one inductive case for each of the remaining four rules. In the base case (atom), for all valuation h such that $\mathbf{B}, h \models \exists v_1 \ldots \exists v_n \phi(i)$, we call the auxiliary lemma allMaps_Correct_Lemma to show that the set allMaps(h, B.Dom) really contains all the maps with domain in h.Keys that give values in B.Dom. In the inductive case where the judgement j is a projection of another derivable judgement j', we recursively call models_Lemma(j',phi,B) for the induction hypothesis that ensures that all (valuations that are) models of j' are in j'.F. Then, the call projection_Lemma(j,j',phi,B) invokes the following auxiliary lemma:

The lemma projection_Lemma assumes, the well-formedness of all its parameters along with, the hypothesis (H1): j is the projection of j' and the fact (as hypothesis (H2)) that j' satisfies the ensures of lemma models, then it ensures that also all valuations that are models of j belongs to j.F. Next, we explain the Dafny proof of projection_Lemma whose code is:⁴

 $^{^4}$ We use to include commented assertions whenever Dafny does not need them as hints, but serve as documentation to the reader, who could check its validity by uncommenting them.

```
var phii := FoI(j.i,phi,B.Sig);
var W := freeVar(phii)-j'.V;
var Y := j' \cdot V - j \cdot V;
var X := freeVar(phii)-j.V;
∀ h: Valuation <T> | valuationModel(h,j,phi,B)
        ensures h in j.F;
        //assert models(B,h,existSq(X,phii));
        assert X = Y + W;
        //assert models(B,h,existSq(Y+W,phii));
        existSq_Sum_Lemma(B, h, Y, W, phii);
        assert models(B,h,existSq(Y,existSq(W,phii)));
        \land setOf(U) = Y \land noDups(U)
                    ∧ setOf(U) ∥ h.Keys
                    \land extVal(h,U,Z).Values \leq B.Dom
                    ^ models(B,extVal(h,U,Z),existSq(W,phii));
        extValDomRange_Lemma(h, U, Z);
        assert extVal(h,U,Z).Keys = j'.V;
        extValallMaps_Lemma(h, U, Z, B);
        assert extVal(h,U,Z) in allMaps(j'.V, B.Dom);
        assert valuationModel(extVal(h,U,Z),j',phi,B);
        //assert extVal(h,U,Z) in j'.F; // by hypothesis (H2)
        //assert h.Keys = j.V;
        projectOfExtVal_Lemma(h, U, Z);
        assert projectVal(extVal(h,U,Z),j.V) = h;
        //assert j.F = ( set f | f in j'.F • projectVal(f,j.V) );
                     // by hypothesis (H1)
        //assert h in j.F;
        3
```

Firstly, we define the variable phii which represents the subformula $\phi(i)$ of index i of the parameter formula ϕ (denoted in code by phi). Then, we define the three sets of variables W,Y and X occurring in $\phi(i)$ and in the judgements j and j'. Next, we proof that any valuation h such that $B, h \models \exists X(\phi(i))$ belongs to j.F. This is the meaning of the \forall -ensures in the code, whose proof is inside the curly brackets that completes the proof. This proof calls five auxiliary lemmas, but it is easy to follow because the assertions after each lemma call explain what they add to prove. By the hypothesis, we have that $B, h \models \exists X(\phi(i))$ where X =Y + W, from here, the auxiliary lemma existSq_Sum_Lemma ensures that $B, h \models$ $\exists Y \exists W(\phi(i))$. Then, by auxiliary lemma existSqSem_Lemma, we basically prove that $B, h[Y \mapsto Z] \models \exists W(\phi(i))$ for some values set of values Z in B. In the code, U is a sequence representing the set Y with no repetitions and disjoint with h.Keys and extVal(h,U,Z) is the Dafny code for h[Y := Z]. After the calls to lemmas extValDomRange_Lemma and extValDomRange_Lemma we prove that hypothesis (H2) can be applied to the mapping $h[Y \mapsto Z]$ so that $h[Y \mapsto Z] \in j'$. F holds. Therefore, its projection $h[Y \mapsto Z] \upharpoonright j.V$, which is proved to coincide with the mapping h (using the auxiliary lemma projectOfExtVal_Lemma), should belong to j.V. The latter is due to hypothesis H1, since by definition of projection j.F is the set of all projection on j.V of all valuations in j'.F. Therefore, $h \in j.F$ is proved. The other three inductive cases –for derivability using (join), (\forall -elimination), and (upward flow)– follows the same lines of the case for (projection) and their code is above omitted. Next, the soundness_Theorem, which states the soundness of the proof system PS, can be easily proved by calling the previous models_Lemma.

18

```
lemma soundness_Theorem <T> (phi: Formula,B: Structure <T>)
requires wfQCSP_Instance(phi,B)
requires is_derivable(J([],{},{}),phi,B)
ensures ¬models(B,map[],phi)
{
var cj := J([],{},{});
models_Lemma(cj,phi,B);
assert ¬valuationModel(map[],cj,phi,B);
}
```

Since the empty judgement is derivable, by models_Lemma, every valuation that is a model of phi belongs to the empty set of valuations. Therefore, every possible valuation with empty domain is not a valuation model of phi. Since the empty function map[] is the only valuation in the set of valuations with empty domain, then (B,map[]) cannot models phi.

Completeness, i.e. the backward direction of Theorem 1, is encoded in the following completeness_Theorem which is proved with the help of the following auxiliary lemma:

Lemma 2 Let (ϕ, \mathbf{B}) be a QCSP instance. Let I_{ϕ} be the index set of ϕ . For each $i \in I_{\phi}$, let F be the set of all valuations such that $\mathbf{B}, h \models \phi(i)$. Then, the judgement $(i, \mathsf{freeVar}(\phi(i)), F)$ is derivable.

We provide a constructive proof of Lemma 2 that associates a judgement to each index i of the formula ϕ . We call it the *canonical judgement*. It is recursively defined by the following function:

```
function canonical_judgement<T> (i: seq<int>, phi: Formula,
                                B: Structure <T>): (cj: Judgement <T>)
  requires wfQCSP_Instance(phi,B)
  requires i in setOfIndex(phi)
  ensures cj.i = i
  ensures cj.V = freeVar(FoI(i,phi,B.Sig))
  ensures wfJudgement(cj,phi,B)
  decreases FoI(i,phi,B.Sig)
ſ
var phii := FoI(i,phi,B.Sig);
indexSubformula_Lemma(i,phi,B.Sig);
match phii
case Atom(R,par) => var F := (set f: Valuation <T> |
                                 f in allMaps(setOf(par),B.Dom)
                                 A HOmap(f,par) in B.I[R]);
                    J(i,setOf(par),F)
var j0 := J(i,j0'.V,j0'.F);
                       var j1 := J(i, j1', V, j1', F);
                       join(j0,j1,phi,B)
case Forall(x,phik) => var j0 := canonical_judgement(i+[0],phi,B);
                       if x in j0.V then dualProjection(x,j0,phi,B)
                                   else J(i,j0.V,j0.F)
case Exists(x,phik) => var j0:= canonical_judgement (i+[0],phi,B);
                       var jp := projection(j0,j0.V-{x},phi,B);
if x in j0.V then J(i,jp.V,jp.F)
                                    else J(i,j0.V,j0.F)
}
```

Note that we name by cj the result produced by the function canonical_judgement. Therefore, the name cj is used in the specification of the function as the shorter name of canonical_judgement(i, phi, B). The well-foundedness of this function is given by the decreasing expression FoI(i,phi,B.Sig), which represents the subformula of phi whose index is i (or $(\phi(i))$). The call to indexSubformula_Lemma ensures that the indexes of the subformulas of phi,phi1,phik, in the succeeding recursive definition given by a match statement, are correct. In that recursive definitions has been ensured to satisfy the respective predicates is_join, is_dualProjection and is_projection (see Section 4). Consequently, Lemma 2 is encoded in the following Dafny lemma

that uses the following function

for representing the set of all valuations that are models of a given formula in a given structure. The lemma canonical_judgement_Lemma is proved by structural induction on phi (we do not show here the proof), with the help of auxiliary lemmas given inductive properties of the definition of setOfValModels for the three different types of composed formulas (And, Forall and Exists) in terms of their component subformula(s). Next, the completeness_Theorem, calling canonical_judgement_Lemma, proves that whenever the sentence phi is not satisfied by the structure B, then the empty judgement of index [] is derivable, indeed it is the cannonical judgement for ([], phi, B,).

The completeness proof proceeds by calling the canonical_judgement_Lemma with canonical judgement associated to the root index [], Dafny infers that this judgement cj is derivable. Moreover, cj.V must be empty and cj.F is the set of all

valuations with empty domain that are valuation models of phi (paired with B) must be empty.

6 Modular Structure

In previous sections, we described the essentials of our formalization and the proofs of the main meta-logical properties: soundness and completeness. However, many technical details and auxiliary properties are proved for that. In our opinion, a modular structure with explicit declarations of the definitions and lemmas that are exported from one module and imported in other module, is essential for refactoring and reuse a large formalization. Moreover, in our experience, modularity demonstrates to be helpful during the development phase. In this section, we give an idea of the whole encoding by describing how it is structured using modules.

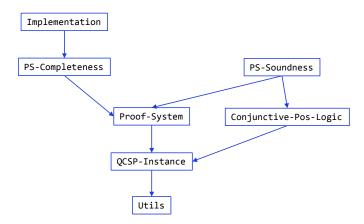


Fig. 2 Module dependencies (w.r.t. include clauses)

Dafny provides modules (keyword module) to group together related entities (such as datatypes, lemmas, functions, predicates, methods, etc.), as well as to control the scope of declarations. and clauses include to include one module in other. In the head of modules, Dafny allows clauses import and export and different qualifiers. In the case of import the qualifier opened allows to use the name of the imported units without the additional prefix of the imported module name. By declaring an export set, a module makes available a subset of its declarations to the module's importers. In the case of export, Dafny supports multiple export sets per module and also allows to name the different exported list. In addition, the qualifiers provides and reveals allows us to export respectively the *specification-part* or also the *body-part* of the exported unit. In other words, each export set indicates the translucency of its exported declarations. For a function, the specification-part includes the function's parameters/results type signature as well as the function's specification, whereas the body-part includes its definition. In Dafny, the verifier always reasons about calls to lemmas (also to methods) in terms of their specifications, never in terms of their bodies. Thus, there would be no difference between

providing and revealing a method or lemma in an export set. For that reason methods and lemmas are disallowed to be mentioned in reveals clauses. Therefore, exported lemmas are always provided, but not revealed. An export set has to be *self consistent*. This means that everything mentioned in the exported declarations must make sense separately. In particular, this means that every symbol that is mentioned in the portions (specification-part or specification-part plus body-part) that are exported must also be part of the export set. The interested reader can find motivations and explanations about the design of the module system of Dafny in [29].

Our formalization is structured in seven modules whose dependencies are described in Figure 2, where the arrows represent the clauses include in each module. The module at the tail of each arrow includes the one at the head of the arrow. The proof system formalization and the proofs of its soundness and completeness consists of six modules: Utils, QCSP-instance, Proof-System, Conjunctive-Pos-Logic, PS-Soundness and PS-Completeness. In addition, the module Implementation contains some additional (verified) methods necessary for implementing the model checker as a web application. More details on the latter are given in Section 7.

Module Utils contains a few auxiliary concepts and properties on sets, sequences and maps that are of general utility. Here we show part of it:

The export list of module Utils reveals a function setOf for the set of elements of a sequence, a predicate noDups for deciding whether a given sequence has duplicates, which has not ensures clauses. However, it provides (but does not reveal) the function allMaps (see Section 4), hence importer modules know its two ensure clauses, but not its body. Module Utils also provides a lemma allMaps_Correct_Lemma, which complements the first ensures clause of allMaps with the backward implication, along with other two lemmas on operations over sets of maps.

In Sections 4 and 5 we explained the most revelant componentes of the four modules QCSP-Instance, Proof-System, PS-Soundness and PS-Completeness. In what follows, we explain the role of the module Conjunctive-Pos-Logic in our formalization. For that, we first give more details about the module QCSP-Instance. This module contains 19 lemmas proving basic properties of the operations on valua-

tions, and also properties on the relation between these operations and the predicate models. Some of this units are auxiliary in the module, to prove the lemmas that are provided to other modules. Next, we show a partial view of the module QCSP-Instance placing emphasis on the relevant elements in the export list to the module Conjunctive-Pos-Logic.

```
module QCSP_Instance {
import opened Utils
export Lemmas_for_Conj_Pos_Logic
       reveals ..., extVal, ...
       provides ..., extValDomRange_Lemma, extValOrder_Lemma,
                 NoFreeVarInExists_Lemma, Exists_Commutes_Lemma
   ... // export lists for other modules
function extVal<T>(f: Valuation<T>, W: seq<Name>, S: seq<T>)
                                                      Valuation <T>
requires |W| = |S| \land noDups(W)
decreases W
{ if W = [] then f else extVal(f[W[0]:=S[0]],W[1..],S[1..]) }
... // other function and predicate definitions
lemma extValDomRange_Lemma<T>(f: Valuation<T>,W: seq<Name>,S: seq<T>)
requires |W| = |S| \land noDups(W)
ensures extVal(f,W,S).Keys = setOf(W) + f.Keys
ensures extVal(f, W, S).Values \subseteq f.Values + setOf(S)
decreases W
⊞{...}
lemma extValOrder_Lemma<T>(k: int,U: seq<Name>,S: seq<T>,f: Valuation<T>)
requires 0 \leq k < |U| = |S| \land noDups(U)
ensures extVal(f, U, S)
          = extVal(f[U[k]:=S[k]], U[..k]+U[k+1..], S[..k]+S[k+1..])
⊞{...}
... // other 15 lemmas
lemma NoFreeVarInExists_Lemma <T>(B: Structure, f: Valuation <T>,
                                  x: Name, beta: Formula)
requires wfStructure(B) \land wfFormula(B.Sig,beta) \land f.Values \subseteq B.Dom
requires x \notin freeVar(beta)
ensures models(B,f,beta) \iff models(B,f,Exists(x,beta))
\boxplus\{\ldots\}
lemma Exists_Commutes_Lemma <T>(x: Name, y: Name, alpha: Formula,
                                f: Valuation <T>, B: Structure <T>)
requires f.Values \subseteq B.Dom
requires models(B, f, Exists(x, Exists(y, alpha)))
ensures models(B, f, Exists(y, Exists(x, alpha)))
\boxplus\{\ldots\}
```

Dotted lines in the export list substitute the elements that are necessary for self consistency, but are not relevant for the present discussion. In other words, 4 of the 19 lemmas proved in QCSP-Instance are basic for proving the 13 lemmas in module Conjunctive-Pos-Logic. The objective of the latter module is to provide the properties of Conjunctive Positive Logic that we need to prove soundness. Indeed, all them are properties about the models of formulas of the form $\exists x_1 \ldots \exists x_n \phi$, which is written in Dafny as existSq(W,phi) where W is the sequence $[x_1 \ldots x_n]$.

The function existSq is defined and exported by module Conjunctive-Pos-Logic, see Figure 3.

```
module Conjunctive_Pos_Logic{
...// import opened clauses
export Lemmas_for_PS_Soundness
  reveals existSq
  provides existSq_ExtVal_Lemma, existSq_Project_Lemma,
             existSq_Sum_Lemma, existSq_And_Lemma,
             existSq_Forall_Lemma, existSq_Exists_Lemma,
             existSqSem_Lemma
function existSq(X: set<Name>, alpha: Formula): Formula
ensures freeVar(existSq(X,alpha)) = freeVar(alpha)-X
ensures ∀ S • wfFormula(S,alpha) ⇒ wfFormula(S,existSq(X,alpha))
if |X| = 0 then alpha else var x : |x in X;
                           Exists(x, existSq(X-{x}, alpha))
}
lemma existSq_And_Lemma <T>(B: Structure <T>, f: Valuation <T>,
                           W: set <Name>, phi: Formula)
requires f.Values \subseteq B.Dom
requires phi. And?
requires models(B,f,existSq(W,phi))
ensures wfFormula(B.Sig,existSq(W ∩ freeVar(phi.0),phi.0))
ensures wfFormula(B.Sig,existSq(W ∩ freeVar(phi.1),phi.1))
ensures models(B,f,existSq(W ∩ freeVar(phi.0), phi.0))
ensures models(B,f,existSq(W ∩ freeVar(phi.1), phi.1))
decreases W
\boxplus\{\ldots\}
... // other 12 lemmas
}
```

Fig. 3 One of the lemmas exported from Conjunctive-Pos-Logic to prove the soundness of proof system PS.

The specification-part of lemma existSq_Distr_And_Lemma is shown in Figure 3 as an example of the kind of properties about models of existSq-formulas that module Conjunctive-Pos-Logic provides to module PS-Soundness. Basically, it proves that

```
if B, f \models \exists x_1 \dots \exists x_n (\phi_0 \land \phi_1),
then B, f \models \exists y_1 \dots \exists y_m (\phi_0) \text{ and } B, f \models \exists z_1 \dots \exists z_k (\phi_1)
```

where $\{y_1, \ldots, y_m\}$ is the set of all variables in $\{x_1, \ldots, x_n\}$ that occur free in ϕ_0 and $\{z_1, \ldots, z_k\}$ is the set of all variables in $\{x_1, \ldots, x_n\}$ that occur free in ϕ_1 . All the lemmas exported (provided) by the module Conjunctive-Pos-Logic are related to (semantic) models of CPL. In particular, the seven lemmas exported by module Conjunctive-Pos-Logic to be imported by the module PS-Soundness, (see export list Lemmas_for_PS_Soundness in Figure 3) assist in the task of proving the lemma models_Lemma that is crucial in the soundness proof, as explained in Section 5. Since models_Lemma (or Lemma 1) refers to an existentially closed formula, the metalogical properties in module Conjunctive-Pos-Logic are related to these existentially closed formulas.

7 Implementation

On the basis of our formalization of proof system PS, we have implemented a verified model checker for Conjunctive Positive Logic. The interface of our model checker asks the user to successively provide the different components of a QCSP-instance (\mathbf{B}, ϕ) , and when completed it returns the result of whether $\mathbf{B} \models \phi$. In this section, we describe our conversion process to generate code and integrate it into the web application. We report on the challenges that arise along this process.

To obtain code from the verified proof system, we basically convert the functions (and predicates) that would take part in the implementation of the web application into methods. By default, Dafny functions (and predicates) are ghost (non-executable), and cannot be called from non-ghost code. Predicates receive the same treatment as functions, they really are boolean functions. To make a function non-ghost, Dafny gives the option, when feasible, to replace the keyword function with the two keywords function method. When a function f defined by an expression E is turned to non-ghost, every function called in the expression E should be turned to non-ghost. Not every expression can be changed from ghost to nonghost, because not every ghost expression is compilable into real code. As a typical example, consider any expression of the form $\forall i: nat \bullet P(i)$ that is body/definition of a predicate Q. If property P does not bound the possible values of i in some way that enables Dafny's heuristics to get a finite set, then the change to predicate method Q raises an error in Dafny that complains: "a quantifier in a nonghost context is allowed only whenever a bounded set of values for its variables (i, in this case) can be computed". In this case, the required function (or predicate) should be implemented by a method whose requires-ensures specification (a.k.a. contract) states that it computes the original function.

The web application checks the well-formedness of the QCSP-instance given by the user, and then compute the canonical judgement to answer "no" if it is empty and "yes" otherwise. Henceforth, at a first glance, we have to convert into non-ghost the predicate wfQCSP_Instance and the function canonical_judgement. As a consequence, all ghost code used in each of these three units has to be also transformed into real code, and the same applies to the ones called from the just transformed into non-ghost. We made this until Dafny has not more complains telling us that "function calls are allowed only in specification context (consider declaring the function as function method)". Dafny marks the affected calls and shows that messages as hover text, which is a valuable help. The predicate wfQCSP_Instance is easily turned non-ghost by simply adding the keyword method in other two predicates and functions definitions. The transformation of function canonical_judgement requires that eight different functions must be also non-ghost. Five of them are solved by simply adding the keyword method. One of the other three functions, which is allMaps, does not satisfy the required conditions for that easy conversion into code, whereas the other two (join and dualProjection) call allMaps. Indeed, the function allMaps makes use of the Hilbert epsilon operator ([32]) declaring var a | a in s, where s is a set, raises the error "to be compilable the value of a

let-such-that-expression must be uniquely determined". To fix this problem, we developed the module Implementation in which we provide a method compute_f for each of the four functions canonical_judgement, allMaps, join and dualProjection as f, and verify the equivalence of each method with the original function. Actually the contract of the methods compute_f specify that it conputes the function f. For example, the contracts of compute_canonical_judgement and compute_allMaps are:

```
method compute_canonical_judgement <T>(i: seq <int>, phi: Formula,
B: Structure <T>)
returns (cj: Judgement <T>)
requires wfQCSP_Instance(phi,B)
requires i in setOfIndex(phi)
ensures cj = canonical_judgement(i,phi,B)
method compute_allMaps <T<sup>(=)</sup>>(keys: set <Name>,values: set <T>)
returns (am: set <map <Name,T>>)
requires values ≠ {}
ensures am = allMaps(keys, values)
```

```
After that, by compiling our formalization, Dafny automatically generates a li-
brary of methods in .NET code (i.e. C#, Visual Basic, and F#). Since .NET does
not have a standard format for inductive datatypes, the data format used by the
Dafny compiler may not agree with the data formats used by other .NET lan-
guages. Therefore, the use of our verified encoding from C\# has required some
data conversions. The compilation process transforms datatypes, such as Structure,
Judgement and Formula, into C# classes. For each constructor C of a datatype D
a class is created named as D_C. All these classes extend a generic abstract one
called Base_D. In addition, there is a class D that has a single constructor with
a parameter of type Base_D. To illustrate this, the datatype Formula has four con-
structors in Dafny specification: Atom, And, Forall and Exists. Dafny generates the
classes Formula, Base_Formula (abstract), Formula_Atom, Formula_And, Formula_Exists
and Formula_Forall. Auxiliary functions are automatically generated to help devel-
opers to handle with the classes. For example, a function is_C is generated for each
constructor c. With the previous classes and auxiliary functions we can instantiate
C\# objects. These can be used as input in methods that require them.
```

The fact that our formalization has already been verified guarantees that every call that satisfies the precondition complies with the postcondition. As a consequence, our web application checks the **requires** clauses before calling the methods. In other words, the only method called by the web application is <code>compute_canonical-judgement</code> whose preconditions are:

```
requires wfQCSP_Instance(phi,B)
requires i in setOfIndex(phi)
```

Hence, before the call compute_canonical-judgement([],pbi,B), we only check that wfQCSP_Instance(phi,B), because [] in setOfIndex(phi) is trivial for any phi.

8 Experience

Our formalization and implementation has been developed in the Dafny IDE ([31]) which lends itself to increase user productivity. The main features of the Dafny IDE are well described in [31]. Our development experience can be termed as

highly positive, mainly because interaction with the tool is easy and it provides good support and helpful information for verification failures, in an agile and fast way. In addition, Dafny supports a number of proof features traditionally found in only interactive proof assistants like Coq or Isabelle/HOL. The task is interesting from the point of view of given a detailed formalization and for debugging the proofs which were previously written with pen and paper in a more imprecise form. Automated proofs often require proving some essential properties that are usually assumed (in the concerned area) without any proof. This is especially the case of many of the lemmas in the module Conjunctive-Pos-Logic which mainly contain logical equivalences that are usually assumed. Moreover, it is feasible that the process of proving some of these properties raised some issue non-properly defined in the formalization. Actually, this was our experience, as we explain in the next paragraph.

There is no doubt that formal verification is useful and important in software development. Details can be subtle and formal verification helps in detecting subtle details that otherwise remain in hiding. The more noteworthy are assumptions that the programmer assume, but she (or he) does not make explicit in the specification. Along the development of our proof many subtle details has been fixed. For example, we forgot to specify, as part of the predicate wfStructure, that the domain of the given structure must be warranted to be non-empty. We realized that when we were not able to proof lemma existSqSem_Lemma in module Conjunctive-Pos-Logic. The interested reader could commented the first line in the body of predicate wfStructure to check that the proof of lemma existSqSem_Lemma is not verified.

Another worthy mistake we made was when we defined the canonical judgement for the universal and existential formulas without taking into account the case when the quantified variable is not in the variables of the judgement. Hence, when we initially tried to prove canonical_judgement_Lemma, the postcondition:

```
ensures cj.F = setOfValmodels(FoI(i,phi,B.Sig),B)
```

couldn't be proved, leading us to see where we were missing.

Among the many interesting lessons learned, we would like to report on the details of the definition of function allMaps in module Utils. For that, we use the function

```
function choose <A>(s: set <A>): A
requires s \neq \{\}
{
var a :| a in s; a
}
```

to encapsulate into this function the application of the Hilbert epsilon operator :|. Otherwise, if we used the operator :|directly in two places: the definition of function allMaps and the proof of lemma allMaps_Correct_Lemma, then each place would choose a different element, which makes the proof of the lemma much harder than putting the expression into a function, because a function produces a unique result for a given argument.

The Dafny formalization, which consists of 1963 lines (including white and commented lines), is structured in seven modules. We take advantage of the import/export mechanism of Dafny for organizing the dependencies between the

module	lines	datatypes	functions	lemmas	methods	proof obl.	secs
Utils	65	0	4	3	0	39	2.90
QCSP-Instance	358	2	8	19	8	697	16.99
Proof-System	218	1	7	4	1	469	14.22
Conjunctive-Pos-Logic	363	0	2	13	0	1,042	46.34
PS-Soundness	288	0	1	8	0	1,004	32.22
PS-Completeness	231	0	4	5	1	698	17.84
Implementation	204	0	0	4	7	256	10.58
TOTAL	1727	3	26	56	17	4,205	141.09

components. Moreover, in Dafny, the exported components can be provided or revealed, which enables to export just the specification, or also the body, of functions and methods.

 Table 1
 Some figures on lines, different Dafny units (datatypes, functions, ...), generated proof obligations, and seconds required for verification, breakdown per module.

In Table 1 we summarize the size of the modules, in terms of the total (noncomment, non-blank) lines of code, the number of datatypes, the number of functions (including predicates), proved lemmas, and methods. The function/predicate methods are counted as methods. The right-most two column respectively reports the number of proof obligations (i.e. queries discharged to Z3) and the seconds required to verify each module by Dafny 2.3.0 for Windows(x64) running by a processor i5-7500 CPU at 2.60GHz 3.40GHz with 16 GB of RAM.

The proof of lemma existSq_Distr_And_Lemma takes about 17,45 seconds, which is the most costly proof, for solving 152 proof obligations. However, the largest set of proof obligations, which consists of 423, is generated by models_Lemma_h is proved in 0,42 seconds. To give some global figures about the proof obligations (PO) generated by lemmas, from the 51 lemmas, there are 18 lemmas that generate at most 20 PO, 16 lemmas that generate from 21 to 60 proof obligations, 21 lemmas that generates from 61 to 250, and only one lemma that produces more than 250 which is the above mentioned models_Lemma_h. Just below it, the lemma canonical_judgement_Lemma produces the number of PO closer to 250, exactly 218, and it is verified in 9,06 seconds.

The amount of effort required to develop the whole system (seven modules of formalization and the web application) is about 250 person-hours.

9 Compliance with Ethical Standards

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