Complexity and Information in Invariant Inference

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This paper addresses the complexity of SAT-based invariant inference, a prominent approach to safety verification. We consider the problem of inferring an inductive invariant of polynomial length given a transition system and a safety property. We analyze the complexity of this problem in a black-box model, called the Hoare-query model, which is general enough to capture algorithms such as IC3/PDR and its variants. An algorithm in this model learns about the system’s reachable states by querying the validity of Hoare triples.

We show that in general an algorithm in the Hoare-query model requires an exponential number of queries. Our lower bound is information-theoretic and applies even to computationally unrestricted algorithms, showing that no choice of generalization from the partial information obtained in a polynomial number of Hoare queries can lead to an efficient invariant inference procedure in this class.

We then show, for the first time, that by utilizing rich Hoare queries, as done in PDR, inference can be exponentially more efficient than approaches such as ICE learning, which only utilize inductiveness checks of candidates. We do so by constructing a class of transition systems for which a simple version of PDR with a single frame infers invariants in a polynomial number of queries, whereas every algorithm using only inductiveness checks and counterexamples requires an exponential number of queries.

Our results also shed light on connections and differences with the classical theory of exact concept learning with queries, and imply that learning from counterexamples to induction is harder than classical exact learning from labeled examples. This demonstrates that the convergence rate of Counterexample-Guided Inductive Synthesis depends on the form of counterexamples.

CCS Concepts:
- Theory of computation → Theory and algorithms for application domains; Program verification;
- Software and its engineering → Formal methods.

Additional Key Words and Phrases: invariant inference, complexity, synthesis, exact learning, property-directed reachability

This technical report is an extended version of:
Yotam M. Y. Feldman, Neil Immerman, Mooly Sagiv, and Sharon Shoham. 2020. Complexity and Information in Invariant Inference. Proc. ACM Program. Lang. 4, POPL, Article 5 (January 2020), 29 pages. https://doi.org/10.1145/3371073

1 INTRODUCTION

The inference of inductive invariants is a fundamental technique in safety verification, and the focus of many works [e.g. Alur et al. 2015; Bradley 2011; Cousot and Cousot 1977; Dillig et al. 2013; Eén et al. 2011; Fedyuikovich and Bodík 2018; McMillan 2003; Srivastava et al. 2013]. The task is to find an assertion I that holds in the initial states of the system, excludes all bad states, and is closed under transitions of the system, namely, the Hoare triple \( \{ I \} \delta \{ I \} \) is valid, where \( \delta \) denotes one step of the system. Such an I overapproximates the set of reachable states and establishes their safety.

The advance of SAT-based reasoning has led to the development of successful algorithms inferring inductive invariants using SAT queries. A prominent example is IC3/PDR [Bradley 2011; Eén et al. 2011], which has led to a significant improvement in the ability to verify realistic hardware systems. Recently, this algorithm has been extended and generalized to software systems [e.g. Bjørner and
Successful SAT-based inference algorithms are typically tricky and employ many clever heuristics. This is in line with the inherent asymptotic complexity of invariant inference, which is hard even with access to a SAT solver [Lahiri and Qadeer 2009]. However, the practical success of inference algorithms calls for a more refined complexity analysis, with the objective of understanding the principles on which these algorithms are based. This paper studies the asymptotic complexity of SAT-based invariant inference through the decision problem of polynomial length inference in the black-box Hoare-query model, as we now explain.

**Inference of polynomial-length CNF.** Naturally, inference algorithms succeed when the invariant they infer is not too long. Therefore, this paper considers the complexity of inferring invariants of polynomial length. We follow the recent trend in invariant inference, advocated in [Bradley 2011; McMillan 2003], to search for invariants in rich syntactical forms, beyond those usually considered in template-based invariant inference [e.g. Alur et al. 2015; Colón et al. 2003; Jeannet et al. 2014; Sankaranarayanan et al. 2004; Srivastava and Gulwani 2009; Srivastava et al. 2013], with the motivation of achieving generality of the verification method and potentially improving the success rate. We thus study the inference of invariants expressed in Conjunctive Normal Form (CNF) of polynomial length. Interestingly, our results also apply to inferring invariants in Disjunctive Normal Form.

**The Hoare-query model.** Our study of SAT-based methods focuses on an algorithmic model called the Hoare-query model. The idea is that the inference algorithm is not given direct access to the program, but performs queries on it. In the Hoare-query model, algorithms repeatedly choose \( \alpha, \beta \) and query for the validity of Hoare triples \( \{\alpha\}\delta\{\beta\} \), where \( \delta \) is the transition relation denoting one step of the system, inaccessible to the algorithm but via such Hoare queries. The check itself is implemented by an oracle, which in practice is a SAT solver. This model is general enough to capture algorithms such as PDR and its variants, and leaves room for other interesting design choices, but does not capture white-box approaches such as abstract interpretation [Cousot and Cousot 1977]. The advantage of this model for a theoretical study is that it enables an information-based analysis, which (i) sidesteps open computational complexity questions, and therefore results in unconditional lower bounds on the computational complexity of SAT-based algorithms captured by the model, and (ii) grants meaning to questions about generalization from partial information we discuss later.

**Results.** This research addresses two main questions related to the core ideas behind PDR, and theoretically analyzes them in the context of the Hoare-query model:

(1) These algorithms revolve around the question of generalization: from observing concrete states (to be excluded from the invariant), the algorithm seeks to produce assertions that hold for all reachable states. The different heuristics in this context are largely understood as clever ways of performing this generalization. The situation is similar in interpolation-based algorithms, only that generalization is performed from bounded safety proofs rather than states. How should generalization be performed to achieve efficient invariant inference?

(2) A key aspect of PDR is the form of SAT checks it uses, as part of relative inductiveness checks, of Hoare triples \( \{\alpha\}\delta\{\beta\} \) in which in general \( \alpha \neq \beta \).\(^1\) Repeated queries of this form are potentially richer than presenting a series of candidate invariants, where the check is \( \{\alpha\}\delta\{\alpha\} \). Is there a benefit in using relative inductiveness beyond inductiveness checks?

\(^1\)For the PDR-savvy: \( \beta \) is typically a candidate clause, and \( \alpha \) is derived from the previous frame.
We analyze these questions in the foundational case of Boolean programs, which is applicable to infinite-state systems through predicate abstraction [Flanagan and Qadeer 2002; Graf and Saidi 1997; Lahiri and Qadeer 2009], and is also a core part of other invariant inference techniques for infinite-state systems [e.g. Hoder and Bjørner 2012; Karbyshev et al. 2017; Komuravelli et al. 2014].

In §6, we answer question 1 with an impossibility result, by showing that no choice of generalization can lead to an inference algorithm using only a polynomial number of Hoare queries. Our lower bound is information-theoretic, and holds even with unlimited computational power, showing that the problem of generalization is chiefly a question of information gathering.

In §7, we answer question 2 in the affirmative, by showing an exponential gap between algorithms utilizing rich \( \{\alpha \} \delta \{\beta \} \) checks and algorithms that perform only inductiveness checks \( \{\alpha \} \delta \{\alpha \} \). Namely, we construct a class of programs for which a simple version of PDR can infer invariants efficiently, but every algorithm learning solely from counterexamples to the inductiveness of candidates requires an exponential number of queries. This result shows, for the first time theoretically, the significance of relative inductiveness checks as the foundation of PDR’s mechanisms, in comparison to a machine learning approach pioneered in the ICE model [Garg et al. 2014, 2016] that infers invariants based on inductiveness checks only (but of course this result does not mean that PDR is always more efficient than every ICE algorithm).

Our results also clarify the relationship between the problem of invariant inference and the classical theory of exact concept learning with queries [Angluin 1987]. In particular, our results imply that learning from counterexamples to induction is harder than learning from positive & negative examples (§8), providing a formal justification to the existing intuition [Garg et al. 2014]. This demonstrates that the convergence rate of learning in Counterexample-Guided Inductive Synthesis [e.g. Jha et al. 2010; Jha and Seshia 2017; Solar-Lezama et al. 2006] depends on the form of examples. We also establish impossibility results for directly applying algorithms from concept learning to invariant inference.

The contributions of the paper are summarized as follows:

- We define the problem of polynomial-length invariant inference, and show it is \( \Sigma^P_2 \)-complete (§4), strengthening the hardness result of template-based abstraction by Lahiri and Qadeer [2009].
- We introduce the Hoare-query model, a black-box model of invariant inference capable of modeling PDR (§5), and study the query complexity of polynomial-length invariant inference in this model.
- We show that in general an algorithm in this model requires an exponential number of queries to solve polynomial-length inference, even though Hoare queries are rich and versatile (§6).
- We also extend this result to a model capturing interpolation-based algorithms (§6.2).
- We show that Hoare queries are more powerful than inductiveness queries (§6.2). This also proves that ICE learning cannot model PDR, and that the extension of the model by Vizel et al. [2017] is necessary.
- We prove that exact learning from counterexamples to induction is harder than exact learning from positive & negative examples, and derive impossibility results for translating some exact concept learning algorithms to the setting of invariant inference (§8).

2 OVERVIEW

Coming up with inductive invariants is one of the most challenging tasks of formal verification—it is often referred to as the “Eureka!” step. This paper studies the asymptotic complexity of automatically inferring CNF invariants of polynomial length, a problem we call polynomial-length inductive invariant inference, in a SAT-based black-box model.
Consider the dilemmas Abby faces when she attempts to develop an algorithm for this problem from first principles. Abby is excited about the popularity of SAT-based inference algorithms. Many such algorithms operate by repeatedly performing checks of Hoare triples of the form $\{\alpha\}\delta\{\beta\}$, where $\alpha, \beta$ are a precondition and postcondition (resp.) chosen by the algorithm in each query and $\delta$ is the given transition relation (loop body). A SAT solver implements the check. We call such checks Hoare queries, and focus in this paper on black-box inference algorithms in the Hoare-query model: algorithms that access the transition relation solely through Hoare queries.

Fig. 1 displays one example program that Abby is interested in inferring an inductive invariant. The state is over $x_1, \ldots, x_n$. The variables $y_1, \ldots, y_n$ are inputs and can change arbitrarily in each step. $c_1, \ldots, c_n$ are immutable, with the assumption that exactly one is true.

![Fig. 1](image_url)

Fig. 1. An example propositional transition system for which we would like to infer an inductive invariant. The state is over $x_1, \ldots, x_n$. The variables $y_1, \ldots, y_n$ are inputs and can change arbitrarily in each step. $c_1, \ldots, c_n$ are immutable, with the assumption that exactly one is true.

2.1 Example: Backward-Reachability with Generalization

How should Abby’s algorithm go about finding inductive invariants? One known strategy is that of backward reachability, in which the invariant is strengthened to exclude states from which bad states may be reachable.\(^2\) Alg. 1 is an algorithmic backward-reachability scheme: it repeatedly checks for the existence of a counterexample to induction (a transition $\sigma, \sigma'$ of $\delta$ from $\sigma \models I$ to $\sigma' \not\models I$), and strengthens the invariant to exclude the pre-state $\sigma$ using the formula $\text{BLOCK}$ returns.

Alg. 1 depends on the choice of $\text{BLOCK}$. The most basic approach is of Alg. 2, which excludes exactly the pre-state, by conjoining to the invariant the negation of the cube of $\sigma$ (the cube is the conjunction

\(^2\)Our results are not specific to backward-reachability algorithms; we use them here for motivation and illustration.
## 2.2 All Generalizations Are Wrong

One simple generalization strategy Abby considers appears in Alg. 3, based on the standard ideas in IC3/PDR [Bradley 2011; Eén et al. 2011] and subsequent developments [e.g. Hoder and Bjørner 2012; Komuravelli et al. 2014]. It starts with the cube (as Alg. 2) and attempts to drop literals, resulting in a smaller conjunction, which many states satisfy; all these states are excluded from the candidate in line 6 of Alg. 1. Hence with this generalization Alg. 1 can exclude many states in each iteration, overcoming the problem with the naive algorithm above. Alg. 3 chooses to drop a literal from the conjunction if no state reachable in at most one step from \( \text{Init} \) satisfies the conjunction even when that literal is omitted (line 4 of Alg. 3); we refer to this algorithm as PDR-1, since it resembles PDR with a single frame.

For example, when in the example of Fig. 1 the algorithm attempts to block the state with \( x = 011 \ldots 1, c = 000 \ldots 1 \), Alg. 3 minimizes the cube to \( d = x_1 \), because no state reachable in at most one step satisfies \( d \), but this is no longer true when another literal is omitted. Conjoining the invariant with \( \neg d \) (in line 6 of Alg. 1) produces a clause of the invariant, \( c_1 \rightarrow \neg x_1 \). In fact, our results show that PDR-1 finds the aforementioned invariant in \( n^2 \) queries.

Yet there is a risk in over-generalization, that is, of dropping too many literals and excluding too many states. In Alg. 1, generalization must not return a formula that other states do not satisfy, or the candidate \( I \) would exclude reachable states and would not be an inductive invariant. Alg. 3 chooses to take the strongest conjunction that does not exclude any state reachable in at most one

| Algorithm 1 | Backward-reachability |
|-------------|------------------------|
| 1: procedure Block-Cube(\( \delta \)) |
| 2: \( I \leftarrow \neg \text{Bad} \) |
| 3: while \( \{ I \} \delta \{ I \} \) not valid do |
| 4: \( \sigma, \sigma' \leftarrow \text{cti}(\delta, I) \) |
| 5: \( d \leftarrow \text{Block}(\delta, \sigma) \) |
| 6: \( I \leftarrow I \land \neg d \) |

| Algorithm 2 | Naive Block |
|-------------|-------------|
| 1: procedure Block-Cube(\( \delta, \sigma \)) |
| 2: return \( \bigwedge \sigma \models p_i \land \bigwedge \neg \sigma \models \neg p_i \) |

| Algorithm 3 | Generalization with Init-Step Reachability |
|-------------|-------------------------------------------|
| 1: procedure Block-PDR-1(\( \delta, \sigma \)) |
| 2: \( d \leftarrow \text{cube}(\sigma) \) |
| 3: for \( l \in \text{cube}(\sigma) \) do |
| 4: \( t \leftarrow d \setminus \{ l \} \) |
| 5: if \( (\text{Init} \implies \neg t) \land \{ \text{Init} \} \delta (\neg t) \) then |
| 6: return \( d \leftarrow t \) |

of all literals that hold in the state; the only state that satisfies \( \text{cube}(\sigma) \) is \( \sigma \) itself, and thus the only one to be excluded from \( I \) in this approach. For example, when Alg. 1 needs to block the state \( x = 011 \ldots 1, c = 000 \ldots 1 \) (this state reaches the bad state \( x = 111 \ldots 1, c = 000 \ldots 1 \)), Alg. 2 does so by conjoining to the invariant the negation of \( \neg x_1 \land x_{n-1} \land x_{n-2} \land \ldots x_1 \land \neg c_n \land \neg c_{n-1} \land \neg c_{n-2} \land \ldots c_1 \), and this is a formula that other states do not satisfy.

Alas, Alg. 1 with blocking by Alg. 2 is not efficient. In essence it operates by enumerating and excluding the states backward-reachable from bad. The number of such states is potentially exponential, making Alg. 2 unsatisfactory. For instance, the example of Fig. 1 requires the exclusion of all states in which \( x \) is odd for every choice of lsb, a number of states exponential in \( n \). The algorithm would thus require an exponential number of queries to arrive at a (CNF) inductive invariant, even though a CNF invariant with only \( n \) clauses exists (as above).

Efficient inference hence requires Abby to exclude more than a single state at each time, namely, to generalize from a counterexample—as real algorithms do. What generalization strategy could Abby choose that would lead to efficient invariant inference?
step; it is of course possible (and plausible) that some states are reachable in two steps but not in one. Alg. 1 with the generalization in Alg. 3 might fail in such cases.

The necessity of generalization, on the one hand, and the problem of over-generalization on the other leads in practice to complex heuristic techniques. Instead of simple backward-reachability with generalization per Alg. 1, PDR never commits to a particular generalization [Eén et al. 2011] through a sequence of frames, which are (in some sense) a sequence of candidate invariants. The clauses resulting from generalization are used to strengthen frames according to a bounded reachability analysis; Alg. 3 corresponds to generalization in the first frame.

Overall, the study of backward-reachability and the PDR-1 generalization leaves us with the question: **Is there a choice of generalization that can be used—in any way—to achieve an efficient invariant inference algorithm?**

In a non-interesting way, the answer is yes, there is a “good” way to generalize: Use Alg. 1, with the following generalization strategy: Upon blocking a pre-state \( \sigma \), compute an inductive invariant of polynomial length, and return the clause of the invariant that excludes \( \sigma \), and this terminates in a polynomial number of steps.

Such generalization is clearly unattainable. It requires (1) perfect information of the transition system, and (2) solving a computationally hard problem, since we show that polynomial-length inference is \( \Sigma_2^P \)-hard (Thm. 4.2). What happens when generalization is computationally unbounded (an arbitrary function), but operates based on partial information of the transition system? Is there a generalization from partial information, be it computationally intractable, that facilitates efficient inference? If such a generalization exists we may wish to view invariant inference heuristics as approximating it in a computationally efficient way.

Similar questions arise in interpolation-based algorithms, only that generalization is performed not from a concrete state, but from a bounded unreachability proof. Still it is challenging to generalize enough to make progress but not too much as to exclude reachable states (or include states from which bad is reachable).

### 2.2.1 Our Results

Our first main result in this paper is that in general, there does not exist a generalization scheme from partial information leading to efficient inference based on Hoare queries. Technically, we prove that even a computationally unrestricted generalization from information gathered from Hoare queries requires an exponential number of queries. This result applies to any generalization strategy and any algorithm using it that can be modeled using Hoare queries, including Alg. 1 as well as more complex algorithms such as PDR. We also extend this lower bound to a model capturing interpolation-based algorithms (Thm. 6.6).

These results are surprising because a-priori it would seem possible, using unrestricted computational power, to devise queries that repeatedly halve the search space, yielding an invariant with a polynomial number of queries (the number of candidates is only exponential because we are interested in invariants up to polynomial length). We show that this is impossible to achieve using Hoare queries.

### 2.3 Inference Using Rich Queries

So far we have established strong impossibility results for invariant inference based on Hoare queries in the general case, even with computationally unrestricted generalization. We now turn to shed some light on the techniques that inference algorithms such as PDR employ in practice. One of the fundamental principles of PDR is the incremental construction of invariants relying on rich Hoare queries. PDR-1 demonstrates a simplified realization of this principle. When PDR-1 considers a clause to strengthen the invariant, it checks the reachability of that individual clause

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3Such a clause exists because \( \sigma \) is backward-reachable from bad states, and thus excluded from the invariant.
from \textit{Init}, rather than the invariant as a whole. This is the Hoare query \{\textit{Init}\}\delta \{\neg t\} in line 4 of Alg. 3, in which, crucially, the precondition is different from the postcondition. The full-fledged PDR is similar in this regard, strengthening a frame according to reachability from the previous frame via relative induction checks [Bradley 2011].

The algorithm in Alg. 2 is fundamentally different, and uses only inductiveness queries \{I\}\delta \{I\}, a specific form of Hoare queries where the precondition and postcondition are the same. Algorithms performing only inductiveness checks can in fact be very sophisticated, traversing the domain of candidates in clever ways. This approach was formulated in the \textit{ICE learning} framework for learning inductive invariants [Garg et al. 2014, 2016] (later extended to general Constrained-Horn Clauses [Ezudheen et al. 2018]), in which algorithms present new candidates based on positive, negative, and implication examples returned by a “teacher” in response to incorrect candidate invariants.\footnote{Our formulation focuses on implication examples—counterexamples to inductiveness queries—and strengthens the algorithm with full information about the set of initial and bad states instead of positive and negative examples (resp.).} The main point is that such algorithms do not perform queries other than inductiveness, and choose the next candidate invariant based solely on the counterexamples to induction showing the previous candidates were unsuitable.

The contrast between the two approaches raises the question: \textit{Is there a benefit to invariant inference in Hoare queries richer than inductiveness?} For instance, to model PDR in the ICE framework, Vizel et al. [2017] extended the framework with relative inductiveness checks, but the question whether such an extension is necessary remained open.

2.3.1 \textit{Our Results}. Our second significant result in this paper is showing an exponential gap between the general Hoare-query model and the more specific inductiveness-query model. To this end, we construct a class of transition systems, including the example of Fig. 1, for which (1) PDR-1, which is a Hoare-query algorithm, infers an invariant in a polynomial number of queries, but (2) every inductiveness-query algorithm requires an \textit{exponential} number of queries, that is, an exponential number of candidates before it finds a correct inductive invariant. This demonstrates that analyzing the reachability of clauses separately can offer an exponential advantage in certain cases. This also proves that PDR cannot be cast in the ICE framework, and that the extension by Vizel et al. [2017] is necessary and strictly increases the power of inference with a polynomial number of queries. To the best of our knowledge, this is not only the first lower bound on ICE learning demonstrating such an exponential gap (also see the discussion in §9), but also the first polynomial upper bound on PDR for a class of systems.

We show this separation on a class of systems constructed using a technical notion of \textit{maximal systems for monotone invariants}. These are systems for which there exists a monotone invariant (namely, an invariant propositional variables appear only negatively) with a linear number of clauses, and the transition relation includes \textit{all} transitions allowed by this invariant. For example, a maximal system can easily be constructed from Fig. 1: this system allows every transition between states satisfying the invariant (namely, between all even \(x\)’s with the same representation), and also every transition between states violating the invariant (namely, between all odd \(x\)’s with the same representation).\footnote{Transitions violating the \(c\) axiom or modifying it are excluded in this modeling.}; a maximal system also includes all the transitions from states that violate that invariant to the states that satisfy it (here, between odd \(x\) and even \(x\) with the same \(c\)). The success of PDR-1 on such systems relies on the small diameter (every reachable state is reachable in one step) and harnesses properties of prime consequences of monotone formulas. In contrast, we show that for inductiveness-query algorithms this class is as hard as the class of \textit{all} programs admitting monotone invariants, whose hardness is established from the results of §2.2.1. For example, from the perspective of inductiveness-query algorithms, the example of Fig. 1, which is a maximal program...
as explained above, is as hard as any system that admits its invariant (and also respects the c axiom and leaves c unchanged). This is because an inductiveness-query algorithm can only benefit from having fewer transitions and hence fewer counterexamples to induction, whereas maximal programs include as many transitions as possible. If an inductiveness query algorithm is to infer an invariant for the example of Fig. 1, it must also be able to infer an invariant for all systems whose transitions are a subset of the transitions of this example. This includes systems with an exponential diameter, as well as systems admitting other invariants, potentially exponentially long. This program illustrates our lower bound construction, which takes all maximal programs for monotone-CNF invariants.

In our lower bound we follow the existing literature on the analysis of inductiveness-query algorithms, which focuses on the worst-case notion w.r.t. potential examples (strong convergence in Garg et al. [2014]). An interesting direction is to analyze inductiveness-query algorithms that exercise some control over the choice of counterexamples to induction, or under probabilistic assumptions on the distribution of examples.

2.4 A Different Perspective: Exact Learning of Invariants with Hoare Queries

This paper can be viewed as developing a theory of exact learning of inductive invariants with Hoare queries, akin to the classical theory of concept learning with queries [Angluin 1987]. The results outlined above are consequences of natural questions about this model: The impossibility of generalization from partial information (§2.2.1) stems from an exponential lower bound on the Hoare-query model. The power of rich Hoare queries (§2.3.1) is demonstrated by an exponential separation between the Hoare- and inductiveness-query models, in the spirit of the gap between concept learning using both equivalence and membership queries and concept learning using equivalence queries alone [Angluin 1990].

The similarity between invariant inference (and synthesis in general) and exact concept learning has been observed before [e.g. Alur et al. 2015; Bshouty et al. 2017; Garg et al. 2014; Jha et al. 2010; Jha and Seshia 2017]. Our work highlights some interesting differences and connections between invariant learning with Hoare, and concept learning with equivalence and membership queries. This comparison yields (im)possibility results for translating algorithms from concept learning with queries to invariant inference with queries. Another outcome is the third significant result of this paper: a proof that learning from counterexamples to induction is inherently harder than learning from examples labeled as positive or negative, formally corroborating the intuition advocated by Garg et al. [2014]. More broadly, the complexity difference between learning from labeled examples and learning from counterexamples to induction demonstrates that the convergence rate of learning in Counterexample-Guided Inductive Synthesis [e.g. Jha et al. 2010; Jha and Seshia 2017; Solar-Lezama et al. 2006] depends on the form of examples. The proof of this result builds on the lower bounds discussed earlier, and is discussed in §8.6

3 BACKGROUND

3.1 States, Transitions Systems, and Inductive Invariants

In this paper we consider safety problems defined via formulas in propositional logic. Given a propositional vocabulary $\Sigma$ that consists of a finite set of Boolean variables, we denote by $F(\Sigma)$ the set of well formed propositional formulas defined over $\Sigma$. A state is a valuation to $\Sigma$. For a state $\sigma$, the cube of $\sigma$, denoted $\text{cube}(\sigma)$, is the conjunction of all literals that hold in $\sigma$. A transition

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6 It may also be interesting to note that one potential difference between classical learning and invariant inference, mentioned by Löding et al. [2016], does not seem to manifest in the results discussed in §2.2.1: the transition systems in the lower bound for inductiveness queries in Corollary 7.11 have a unique inductive invariant, and still the problem is hard.
system is a triple \( TS = (Init, \delta, Bad) \) such that \( Init, Bad \in \mathcal{F}(\Sigma) \) define the initial states and the bad states, respectively, and \( \delta \in \mathcal{F}(\Sigma \cup \Sigma') \) defines the transition relation, where \( \Sigma' = \{ x' \mid x \in \Sigma \} \) is a copy of the vocabulary used to describe the post-state of a transition. A class of transition systems, denoted \( \mathcal{P}_i \), is a set of transition systems. A transition system \( TS \) is safe if all the states that are reachable from the initial states via steps of \( \delta \) satisfy \( \neg Bad \). An inductive invariant for \( TS \) is a formula \( I \in \mathcal{F}(\Sigma) \) such that \( Init \implies I, I \land \delta \implies I', \) and \( I \implies \neg \text{Bad} \), where \( I' \) denotes the result of substituting each \( x \in \Sigma \) for \( x' \in \Sigma' \) in \( I \), and \( \varphi \implies \psi \) denotes the validity of the formula \( \varphi \rightarrow \psi \). In the context of propositional logic, a transition system is safe if and only if it has an inductive invariant. When \( I \) is not inductive, a counterexample to induction is a pair of states \( \sigma, \sigma' \) such that \( \sigma, \sigma' \models I \land \delta \land \neg I' \) (where the valuation to \( \Sigma' \) is taken from \( \sigma' \)).

The classes \( \text{CNF}_n, \text{DNF}_n \) and \( \text{Mon-CNF}_n \). \( \text{CNF}_n \) is the set of propositional formulas in Conjunctive Normal Form (CNF) with at most \( n \) clauses (disjunction of literals). \( \text{DNF}_n \) is likewise for Disjunctive Normal Form (DNF), where \( n \) is the maximal number of cubes (conjunctions of literals). \( \text{Mon-CNF}_n \) is the subset of \( \text{CNF}_n \) in which all literals are negative.

### 3.2 Invariant Inference Algorithms

In this section we briefly provide background on inference algorithms that motivate our theoretical development in this paper. The main results of the paper do not depend on familiarity with these algorithms or their details; this (necessarily incomprehensive) “inference landscape” is presented here for context and motivation for defining the Hoare-query model (§5), studying its complexity and the feasibility of generalization (§6), and analyzing the power of Hoare queries compared to inductiveness queries (§7). We allude to specific algorithms in motivating each of these sections.

#### IC3/PDR

IC3/PDR maintains a sequence of formulas \( F_0, F_1, \ldots \), called frames, each of which can be understood as a candidate inductive invariant. The sequence is gradually modified and extended throughout the algorithm’s run. It is maintained as an approximate reachability sequence, meaning that (1) \( Init \implies F_0 \), (2) \( F_j \implies F_{j+1} \), (3) \( F_j \land \delta \implies (F_{j+1})' \), and (4) \( F_j \implies \neg \text{Bad} \). These properties ensure that \( F_j \) overapproximates the set of states reachable in \( j \) steps, and that the approximations contain no bad states. (We emphasize that \( F_j \implies \neg \text{Bad} \) does not imply that a bad state is unreachable in any number of states.) The algorithm terminates when one of the frames implies its preceding frame \( (F_j \implies F_{j-1}) \), in which case it constitutes an inductive invariant, or when a counterexample trace is found. In iteration \( N \), a new frame \( F_N \) is added to the sequence. One way of doing so is by initializing \( F_N \) to \( true \), and strengthening it until it excludes all bad states. Strengthening is done by blocking bad states: given a bad state \( \sigma_b \models F_N \land \text{Bad} \), the algorithm strengthens \( F_{N-1} \) to exclude all \( \sigma_b \)'s pre-states—states that satisfy \( F_{N-1} \land \delta \land (\text{cube}(\sigma_b))' \)—one by one (thereby demonstrating that \( \sigma_b \) is unreachable in \( N \) steps). Blocking a pre-state \( \sigma_a \) from frame \( N - 1 \) is performed by a recursive call to block its own pre-states from frame \( N - 2 \), and so on. If this process reaches a state from \( Init \), the sequence of states from the recursive calls constitutes a trace reaching \( \text{Bad} \) from \( Init \), which is a counterexample to safety. Alternatively, when a state \( \sigma \) is successfully found to be unreachable from \( F_{j-1} \) in one step, i.e., \( F_{j-1} \land \delta \land (\text{cube}(\sigma_b))' \) is unsatisfiable, frame \( F_j \) is strengthened to reflect this fact. Aiming for efficient convergence (see §2.1), PDR chooses to generalize, and exclude more states. A basic form of generalization is performed by dropping literals from \( \text{cube}(\sigma) \) as long as the result \( t \) is still unreachable from \( F_{j-1} \), i.e., \( F_{j-1} \land \delta \land t' \) is still unsatisfiable. This is very similar to PDR-1 above (§2.2), where \( F_{j-1} \) was always \( F_0 = \text{Init} \). Often inductive generalization is used, dropping literals as long as \( F_{j-1} \land \neg t \land \delta \land t' \), reading that \( \neg t \) is inductive relative to \( F_{j-1} \), which can drop more literals than basic generalization. A core optimization of PDR is pushing, in which a frame \( F_j \) is “opportunistically” strengthened with a clause \( \alpha \) from \( F_{j-1} \), if \( F_{j-1} \) is already sufficiently strong to show that \( \alpha \) is unreachable in \( F_j \).
For a more complete presentation of PDR and its variants as a set of abstract rules that may be applied nondeterministically see e.g. Gurflinkel and Ivrri [2015]; Hoder and Bjørner [2012]. The key point from the perspective of this paper is that the algorithm and its variants access the transition relation δ in a very specific way, checking whether some α is unreachable in one step of δ from the set of states satisfying a formula F (or those satisfying F ∧ α), and obtains a counterexample when it is reachable (see also Vizel et al. [2017]). Crucially, other operations (e.g., maintaining the frames, checking whether F_j \implies F_{j-1}, etc.) do not use δ. We will return to this point when discussing the Hoare-query model, which can capture IC3/PDR (§5).

**ICE.** The ICE framework [Garg et al. 2014, 2016] (later extended to general Constrained-Horn Clauses [Ezudheen et al. 2018]), is a learning framework for inferring invariants from positive, negative and implication counterexamples. We now review the framework using the original terminology and notation; later in the paper we will use a related formulation that emphasizes the choice of candidates (in §7.1).

In ICE learning, the teacher holds an unknown target (P, N, R), where P, N ⊆ D, R ⊆ D × D are sets of examples. The learner’s goal is to find a hypothesis H ∈ C s.t. P ⊆ H, N ∩ H = ∅, and for each (x, y) ∈ R, x ∈ H ⇒ y ∈ H. The natural way to cast inference in this framework is, given a transition system (Init, δ, Bad) and a set of candidate invariants L, to take D as the set of program states, P a set of reachable states including Init, N a set of states including Bad from which a safety violation is reachable, R the set of transitions of δ, and C = L. Iterative ICE learning operates in rounds. In each round, the learner is provided with a sample—(E, B, I) s.t. E ⊆ P, B ⊆ N, I ⊆ R—and outputs a hypothesis H ∈ C. The teacher returns that the hypothesis is correct, or extends the sample with an example showing that H is incorrect. The importance of implication counterexamples is that they allow implementing a teacher using a SAT/SMT solver without “guessing” what a counterexample to induction indicates [Garg et al. 2014; Løding et al. 2016]. Examples of ICE learning algorithms include Houdini [Flanagan and Leino 2001] and symbolic abstraction [Reps et al. 2004; Thakur et al. 2015], as well as designated algorithms [Garg et al. 2014, 2016]. Theoretically, the analysis of Garg et al. [2014] focuses on strong convergence of the learner, namely, that the learner can always reach a correct concept, no matter how the teacher chooses to extend samples between rounds. In this work, we will be interested in the number of rounds the learner performs. We will say that the learner is strongly-convergent with round-complexity r if for every ICE teacher, the learner finds a correct hypothesis in at most r rounds, provided that one exists. We extend this definition to a class of target descriptions in the natural way.

**Interpolation.** The idea of interpolation-based algorithms, first introduced by McMillan [2003], is to generalize proofs of bounded unreachability into elements of a proof of unbounded reachability, utilizing Craig interpolation. Briefly, this works as follows: encode a bounded reachability from a set of states F in k steps, and use a SAT solver to find that this cannot reach Bad. When efficient interpolation is supported in the logic and solver, the SAT solver can produce an interpolant C: a formula representing a set of states that (i) overapproximates the set of states reachable from F in k_1 steps, and still (ii) cannot reach Bad in k_2 steps (any choice k_1 + k_2 = k is possible). Thus C overapproximates concrete reachability from F without reaching a bad state, although both these facts are known in only a bounded number of steps. The hope is that C would be a useful generalization to include as part of the invariant. The original algorithm [McMillan 2003] sets some k as the current unrolling bound, starts with F = Init, obtains an interpolant C with k_1 = 1, k_2 = k - 1, sets F ← F ∨ C and continues in this fashion, until an inductive invariant is found, or Bad becomes reachable in k steps from F, in which case k is incremented and the algorithm is restarted. The use of interpolation and generalization from bounded unreachability has been used in many works since [e.g. Henzinger et al. 2004; Jhala and McMillan 2007; McMillan 2006; Vizel and Grumberg...
2009; Vizel et al. 2013]. Combining ideas from interpolation and PDR has also been studied [e.g. Vizel and Gurfinkel 2014]. The important point for this paper is that many interpolation-based algorithms only access the transition relation when checking bounded reachability (from some set of states \( \alpha \) to some set of states \( \beta \)), and extracting interpolants when the result is unreachable. We will return to this point when discussing the interpolation-query model, which aims to capture interpolation-based algorithms (§6.2).

4 POLYNOMIAL-LENGTH INVARIANT INFERENCE

In this section we formally define the problem of polynomial-length invariant inference for CNF formulas, which is the focus of this paper. We then relate the problem to the problem of inferring DNF formulas with polynomially many cubes via duality (see Appendix A), and focus on the case of CNF in the rest of the paper.

Our object of study is the problem of polynomial-length inference:

**Definition 4.1 (Polynomial-Length Inductive Invariant Inference).** The polynomial-length inductive invariant inference problem (invariant inference for short) for a class of transition systems \( P \) and a polynomial \( p(n) = \Omega(n) \) is the problem: Given a transition system \( TS \in P \) over \( \Sigma \), decide whether there exists an inductive invariant \( I \in \text{CNF}_{p(n)} \) for \( TS \), where \( n = |\Sigma| \).

**Notation.** In the sequel, when considering the polynomial-length inductive invariant inference problem of a transition system \( TS = (\text{Init}, \delta, \text{Bad}) \in P \), we denote by \( \Sigma \) the vocabulary of \( \text{Init}, \text{Bad} \) and \( \delta \). Further, we denote \( n = |\Sigma| \).

**Complexity.** The complexity of polynomial-length inference is measured in \( |TS| = |\text{Init}| + |\delta| + |\text{Bad}| \). Note that the invariants are required to be polynomial in \( n = |\Sigma| \).

\( \text{CNF}_{p(n)} \) is a rich class of invariants. Inference in more restricted classes can be solved efficiently. For example, when only conjunctive candidate invariants are considered, and \( P \) is the set of all propositional transition systems, the problem can be decided in a polynomial number of SAT queries through the Houdini algorithm [Flanagan and Leino 2001; Lahiri and Qadeer 2009]. Similar results hold also for CNF formulas with a constant number of literals per clause (by defining a new predicate for each of the polynomially-many possible clauses and applying Houdini), and for CNF formulas with a constant number of clauses (by translating them to DNF formulas with a constant number of literals per cube and applying the dual procedure). However, a restricted class of invariants may miss invariants for some programs and reduces the generality of the verification procedure. Hence in this paper we are interested in the richer class of polynomially-long CNF invariants. In this case the problem is no longer tractable even with a SAT solver:

**Theorem 4.2.** Let \( P \) be the set of all propositional transition systems. Then polynomial-length inference for \( P \) is \( \Sigma_2^P \)-complete, where \( \Sigma_2^P = \text{NP}^{\text{SAT}} \) is the second level of the polynomial-time hierarchy.

We defer the proof to §6.1.1.

We note that polynomial-length inference can be encoded as specific instances of template-based inference; the \( \Sigma_2^P \)-hardness proof of Lahiri and Qadeer [2009] uses more general templates and therefore does not directly imply the \( \Sigma_2^P \)-hardness of polynomial-length inference. Lower bounds on polynomial-length inference entail lower bounds for template-based inference.

**Remark 4.1.** In the above formulation, an efficient procedure for deciding safety does not imply polynomial-length inference is tractable, since the program may be safe, but all inductive invariants may be too long. To overcome this technical quirk, we can consider a promise problem [Goldreich 2006] variant of polynomial-length inference:

Given a transition system \( TS \in P \).
• (Completeness) If TS has an inductive invariant \( I \in \text{CNF}_{p(n)} \), the algorithm must return yes.
• (Soundness) If TS is not safe the algorithm must return no.

Other cases, including the case of safety with an invariant outside \( \text{CNF}_{p(n)} \), are not constrained. An algorithm deciding safety thus solves also this problem. All the results of this paper apply both to the standard version above and the promise problem: upper bounds on the standard version trivially imply upper bounds on the promise problem, and in our lower bounds we use transition systems that are either (i) safe and have an invariant in \( \text{CNF}_{p(n)} \), or (ii) unsafe.

5 INVARIANT INFERENCES WITH QUERIES AND THE HOARE QUERY MODEL

In this paper we study algorithms for polynomial-length inference through black-box models of inference with queries. In this setting, the algorithm accesses the transition relation through (rich) queries, but cannot read the transition relation directly. Our main model is of Hoare-query algorithms, which query the validity of a postcondition from a precondition in one step of the system. Hoare-query algorithms faithfully capture a large class of SAT-based invariant inference algorithms, including PDR and related methods.

A black-box model of inference algorithms facilitates an analysis of the information of the transition relation the algorithm acquires. The advantage is that such an information-based analysis sidesteps open computational complexity questions, and therefore results in unconditional lower bounds on the computational complexity of SAT-based algorithms captured by the model. Such an information-based analysis is also necessary for questions involving unbounded computational power and restricted information, in the context of computationally-unrestricted bounded-reachability generalization (see §6.3).

In this section we define the basic notions of queries and query-based inference algorithms. We also define the primary query model we study in the paper: the Hoare-query model. In the subsequent sections we introduce and study additional query models: the interpolation-query model (§6.2), and the inductiveness-query model (§7.1).

Inference with queries. We model queries of the transition relation in the following way: A query oracle \( Q \) is an oracle that accepts a transition relation \( \delta \), as well as additional inputs, and returns some output. The additional inputs and the output, together also called the interface of the oracle, depend on the query oracle under consideration. A family of query oracles \( Q \) is a set of query oracles with the same interface. We consider several different query oracles, representing different ways of obtaining information about the transition relation.

Definition 5.1 (Inference algorithm in the query model). An inference algorithm from queries, denoted \( \mathcal{A}_Q(\text{Init}, \text{Bad}, [\delta]) \), is defined w.r.t. a query oracle \( Q \) and is given:
  - access to the query oracle \( Q \),
  - the set of initial states (\( \text{Init} \)) and bad states (\( \text{Bad} \));
  - the transition relation \( \delta \), encapsulated—hence the notation \([\delta]\)—meaning that the algorithm cannot access \( \delta \) (not even read it) except for extracting its vocabulary; \( \delta \) can only be passed as an argument to the query oracle \( Q \).

\( \mathcal{A}_Q(\text{Init}, \text{Bad}, [\delta]) \) solves the problem of polynomial-length invariant inference for \( (\text{Init}, \delta, \text{Bad}) \).

The Hoare-query model. Our main object of study in this paper is the Hoare-query model of invariant inference algorithms. It captures SAT-based invariant inference algorithms querying the behavior of a single step of the transition relation at a time.

Definition 5.2 (Hoare-Query Model). For a transition relation \( \delta \) and input formulas \( \alpha, \beta \in \mathcal{F}(\Sigma) \), the Hoare-query oracle, \( \mathcal{H}(\delta, \alpha, \beta) \), returns false if \((\alpha \land \delta \land \neg \beta') \in \text{SAT}\); otherwise it returns true.
An algorithm in the Hoare-query model, also called a Hoare-query algorithm, is an inference from queries algorithm expecting the Hoare query oracle.

Intuitively, a Hoare-query algorithm gains access to the transition relation, \( \delta \), exclusively by repeatedly choosing \( \alpha, \beta \in \mathcal{F}(\Sigma) \), and calling \( \mathcal{H}(\delta, \alpha, \beta) \).

If we are using a SAT solver to compute the Hoare-query, \( \mathcal{H}(\delta, \alpha, \beta) \), then when the answer is false, the SAT solver will also produce a counterexample pair of states \( \sigma, \sigma' \) such that \( \sigma, \sigma' \models \alpha \land \delta \land \neg \beta' \).

We observe that using binary search, a Hoare-query algorithm can do the same:

**Lemma 5.3.** Whenever \( \mathcal{H}(\delta, \alpha, \beta) = \text{false} \), a Hoare-query algorithm can find \( \sigma, \sigma' \) such that \( \sigma, \sigma' \models \alpha \land \delta \land \neg \beta' \) using \( n = |\Sigma| \) Hoare queries.

**Proof.** For each \( x_i \in \Sigma \cup \Sigma' \), if \( x_i \in \Sigma \), conjoin it to \( \alpha \), else to \( \beta \), and check whether \( \mathcal{H}(\delta, \alpha_i, \beta_i) \) is still false. If it is, continue to \( x_{i+1} \); otherwise flip \( x_i \) and continue to \( x_{i+1} \). \( \square \)

**Example: PDR as a Hoare-query algorithm.** The Hoare-query model captures the prominent PDR algorithm, facilitating its theoretical analysis. As discussed in §3.2, PDR accesses the transition relation via checks of unreachability in one step and counterexamples to those checks. These operations are captured in the Hoare query model by checking \( \mathcal{H}(\delta, F, \alpha) \) or \( \mathcal{H}(\delta, F \land \alpha, \alpha) \) (for the algorithm’s choice of \( F, \alpha \in \mathcal{F}(\Sigma) \)), and obtaining a counterexample using a polynomial number of Hoare queries, if one exists (Lemma 5.3). Furthermore, the Hoare-query model is general enough to express a broad range of PDR variants that differ in the way they use such checks but still access the transition relation only through such queries.

The Hoare-query model is not specific to PDR. It also captures algorithms in the ICE learning model [Garg et al. 2014], as we discuss in §7.1, and as result can model algorithms captured by the ICE model (see §3.2). In §7.2 we show that the Hoare-query model is in fact strictly more powerful than the ICE model.

**Remark 5.1.** Previous black-box models for invariant inference [Garg et al. 2014] encapsulated access also to Init, Bad. In our model we encapsulate only access to \( \delta \), since (1) it is technically simpler, (2) a simple transformation can make Init, Bad uniform across all programs, embedding the differences in the transition relation; indeed, our constructions of classes of transition systems in this paper are such that Init, Bad are the same in all transition systems that share a vocabulary, hence Init, Bad may be inferred from the vocabulary. (Unrestricted access to Init, Bad is stronger, thus lower bounds on our models apply also to models restricting access.)

**Complexity.** Focusing on information, we do not impose computational restrictions on the algorithms, and only count the number of queries the algorithm performs to reveal information of the transition relation. In particular, when establishing lower bounds on the query complexity, we even consider algorithms that may compute non-computable functions. However, whenever we construct algorithms demonstrating upper bounds on query complexity, these algorithms in fact have polynomial time complexity, and we note this when relevant.

Given a query oracle and an inference algorithm that uses it, we analyze the number of queries the algorithm performs as a function of \( n = |\Sigma| \), in a worst-case model w.r.t. to possible transition systems over \( \Sigma \) in the class of interest.

The definition is slightly more complicated by considering, as we do later in the paper, query-models in which more than one oracle exists, i.e., an algorithm may use any oracle from a family of query oracles. In this case, we analyze the query complexity of an algorithm in a worst-case model w.r.t. the possible query oracles in the family as well.

Formally, the query complexity is defined as follows:
Definition 5.4 (Query Complexity). For a class of transitions systems $\mathcal{P}$, the query complexity of (a possibly computationally unrestricted) $\mathcal{A}$ w.r.t. a query oracle family $\mathcal{Q}$ is defined as

$$q_{\mathcal{A}}^{\mathcal{Q}}(n) = \sup_{Q \in \mathcal{Q}} \sup_{(\text{Init}, \delta, \text{Bad}) \in \mathcal{P}, |\Sigma| = n} \#\text{query}(\mathcal{A}^Q(\text{Init}, \text{Bad}, [\delta]))$$

where $\#\text{query}(\mathcal{A}^Q(\text{Init}, \text{Bad}, [\delta]))$ is the number of times the algorithm accesses $Q$ given this oracle and the input. (These numbers might be infinite.)

The query complexity in the Hoare-query model is $q_{\mathcal{A}}^{\{H\}}(n)$.

Remark 5.2. In our definition, query complexity is a function of the size of the vocabulary $n = |\Sigma|$, but not of the size of the representation of the transition relation $|\delta|$. This reflects the fact that an algorithm in the black-box model does not access $\delta$ directly. In Appendix B we discuss the complexity w.r.t. $|\delta|$ as well. The drawback of such a complexity measure is that learning $\delta$ itself becomes feasible, undermining the black-box model. Efficiently learning $\delta$ is possible when using unlimited computational power and exponentially-long queries. However, whether the same holds when using unlimited computational power with only polynomially-long queries is related to open problems in classical concept learning.

6 THE INFORMATION COMPLEXITY OF HOARE-QUERY ALGORITHMS

In this section we prove an information-based lower bound on Hoare-query invariant inference algorithms, and also extend the results to algorithms using interpolation, another SAT-based operation. We then apply these results to study the role of information in generalization as part of inference algorithms.

6.1 Information Lower Bound for Hoare-Query Inference

We show that a Hoare-query inference algorithm requires $2^{\Omega(n)}$ Hoare-queries in the worst case to decide whether a CNF invariant of length polynomial in $n$ exists. (Recall that $n$ is a shorthand for $|\Sigma|$, the size of the vocabulary of the input transition system.) This result applies even when allowing the choice of queries to be inefficient, and when allowing the queries to use exponentially-long formulas. It provides a lower bound on the time complexity of actual algorithms, such as PDR, that are captured by the model. Formally:

**Theorem 6.1.** Every Hoare-query inference algorithm $\mathcal{A}^H$ deciding polynomial-length inference for the class of all propositional transition systems has query complexity of $2^{\Omega(n)}$.

The rest of this section proves a strengthening of this theorem, for a specific class of transition systems (which we construct next), for any class of invariants that includes monotone CNF, and for computationally-unrestricted algorithms:

**Theorem 6.2.** Every Hoare-query inference algorithm $\mathcal{A}^H$, even computationally-unrestricted, deciding invariant inference for the class of transition systems $\mathcal{P}_{\Sigma^p}$ (§6.1.1) and for any class of target invariants $\mathcal{L}$ s.t. Mon-CNF$_n \subseteq \mathcal{L}$ has query complexity of $2^{\Omega(n)}$.

(That classes containing Mon-CNF$_n$ are already hard becomes important in §7.)

6.1.1 A Hard Class of Transition Systems. In this section we construct a $\mathcal{P}_{\Sigma^p}$, a hard class of transition systems, on which we prove hardness results.

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Here we extend the definition of polynomial-length invariant inference to $\mathcal{L}$ instead of CNF$_{p(n)}$.
The QBF₂ problem. The construction of $\mathcal{P}_{\Sigma = P}^k$ follows the $\Sigma_k = P$-complete problem of QBF₂ from classical computational complexity theory. In this problem, the input is a quantified Boolean formula $\exists \overline{y}. \forall \overline{x}. \phi(\overline{x}, \overline{y})$ where $\phi$ is a Boolean (quantifier-free) formula, and the problem of QBF₂ is to decide whether the quantified formula is true, namely, there exists a Boolean assignment to $\overline{y}$ s.t. $\phi(\overline{x}, \overline{y})$ is true for every Boolean assignment to $\overline{x}$.

The class $\mathcal{P}_{\Sigma = P}^k$. For each $k \in \mathbb{N}$, we define $\mathcal{P}_{\Sigma = P}^k$. Finally, $\mathcal{P}_{\Sigma = P} = \bigcup_{k \in \mathbb{N}} \mathcal{P}_{\Sigma = P}^k$.

Let $k \in \mathbb{N}$. For each formula $\exists \overline{y}. \forall \overline{x}. \phi(\overline{y}, \overline{x})$, where $\overline{y} = y_1, \ldots, y_k$, $\overline{x} = x_1, \ldots, x_k$ are variables and $\phi$ is a quantifier-free formula over the variables $\overline{x}$, we define a transition system $TS^\phi = (Init_k, \delta^\phi_k, Bad_k)$. Intuitively, it iterates through $\overline{y}$ lexicographically and, for each $\overline{y}$ it iterates lexicographically through $\overline{x}$ and checks if all assignments to $\overline{x}$ satisfy $\phi(\overline{y}, \overline{x})$. If no such $\overline{y}$ is found, this is an error. More formally,

1. $\Sigma_k = \{y_1, \ldots, y_k, x_1, \ldots, x_k, a, b, e\}$.
2. $Init_k(\overline{y}) \equiv \overline{y} = \overline{0} \land \overline{x} = \overline{0} \land \neg a \land b \land \neg e$.
3. $Bad_k(\overline{y}) \equiv e$.
4. $\delta^\phi_k(\overline{y}, \overline{x})$: evaluate $\phi(\overline{y}, \overline{x})$, and perform the following changes (at a single step): If the result is false, set $a$ to true. If $\overline{x} = \overline{1}$ and $a$ is still false, set $b$ to false. If in the pre-state $\overline{x} = \overline{1}$, increment $\overline{y}$ lexicographically, reset $a$ to false, and set $\overline{x} = \overline{0}$; otherwise increment $\overline{x}$ lexicographically. If in the pre-state $\overline{y} = \overline{1}$, set $e$ to $b$. (Intuitively, $a$ is false as long as no falsifying assignment to $\overline{x}$ has been encountered for the current $\overline{y}$, $b$ is true as long as we have not yet encountered a $\overline{y}$ for which there is no falsifying assignment.)

We denote the resulting class of transition systems $\mathcal{P}_{\Sigma = P}^k = \{TS^\phi \mid \phi = \phi(y_1, \ldots, y_k, x_1, \ldots, x_k)\}$.

The following lemma relates the QBF₂ problem for $\phi$ to the inference problem of $TS^\phi$:

**Lemma 6.3.** Let $TS^\phi \in \mathcal{P}_{\Sigma = P}^k$. Then $TS^\phi$ is safe iff it has an inductive invariant in Mon-CNF₂k+1 iff the formula $\exists \overline{y}. \forall \overline{x}. \phi(\overline{y}, \overline{x})$ is true.

**Proof.** There are two cases:

- If $\exists \overline{y}. \forall \overline{x}. \phi(\overline{y}, \overline{x})$ is true, let $\overline{v}$ be the first valuation for $\overline{y}$ that realizes the existential quantifiers. Then the following is an inductive invariant for $TS^\phi$:

$$I = \neg e \land (b \rightarrow \overline{y} \leq \overline{v}) \land ((b \land a) \rightarrow \overline{y} < \overline{v})$$

(2)

where the lexicographic constraint is expressed by the following recursive definition on $\overline{y}[d] = (y_1, \ldots, y_d)$, $\overline{v}[d] = (v_1, \ldots, v_d)$:

$$\overline{y}[d] < \overline{v}[d] \overset{\text{def}}{=} \begin{cases} 
\neg y_d \lor (\overline{y}[d-1] < \overline{v}[d-1]) & v_d = \text{true} \\
\neg y_d \land (\overline{y}[d-1] < \overline{v}[d-1]) & v_d = \text{false}
\end{cases}$$

and $\overline{y} \leq \overline{v} \overset{\text{def}}{=} \overline{y} < (\overline{v} + 1)$ (or true if $\overline{v} = \overline{1}$).

$I \in$ Mon-CNF₂k+1: Note that $\overline{y}[k] < \overline{v}[k]$ can be written in CNF with at most $n$ clauses: in the first case a literal is added to each clause, and in the second another clause is added. Thus $I$ can be written in CNF with at most $2k + 1$ clauses. Further, the literals of $\overline{y}$ appear only negatively in $\overline{y}[k] < \overline{v}[k]$, and hence also in $I$. The other literals ($\neg e, \neg a, \neg b$) also appear only negatively in $I$. Hence, $I$ is monotone.

$I$ is indeed an inductive invariant: initiation and safety are straightforward. For consecution, consider a valuation to $\overline{y}$ in a pre-state satisfying the invariant. (We abuse notation and refer to the valuation by $\overline{y}$.) There are three cases:
We begin with some notation. Running on input \(\varphi\) there exist two formulas \(\psi_1, \psi_2\) at least \(2\) that the number of Hoare queries performed by \(\alpha\) opposed to the result \(\text{true}\). Intuitively, such responses are less informative and rule out less transition relations, because they merely indicate the existence of a single counterexample to a Hoare triple, \(\text{false}\). The construction uses the path the algorithm takes when all Hoare queries return \(\text{true}\), and \(\text{false}\) after a step, and once we finish iterating through \(\varphi\) we set \(\text{false}\) immediately.

The claim follows.

- If \(\exists y. \forall x. \phi(y, x)\) is not true, then \(TS^{\phi}\) is not safe (and thus does not have an inductive invariant of any length). This is because for every valuation of \(y\) a violating \(x\) is found, turning \(\alpha\) to \(\text{true}\), and \(b\) never turns to \(\text{false}\), so after iterating through all possible \(y\)'s \(e\) will become true.

Before we turn to prove Thm. 6.2 and establish a lower bound on the query complexity in the Hoare model, we note that this construction also yields the computational hardness mentioned in §4:

\begin{proof}[Proof of Thm. 4.2.]

The upper bound is straightforward: guess an invariant in CNF \(p(n)\) and check it. For the lower bound, use the reduction outlined above: given \(\phi(y_1, \ldots, y_k, x_1, \ldots, x_k)\), construct \(TS^{\phi}\). Note that the vocabulary size, \(n\), is \(2k + 3\), and the invariant, when exists, is of length at most \(2k + 1 \leq n\).\(^6\) The reduction is polynomial as the construction of \(TS^{\phi}\) (and \(n\)) from \(\phi\) is polynomial in \(k\) and \(|\phi|\): note that lexicographic incrementation can be performed with a propositional formula of polynomial size.
\end{proof}

\subsection{Lower Bound’s Proof}

We now turn to prove Thm. 6.2. Given an algorithm with polynomial query complexity, the proof constructs two transition system: one that has a polynomial-length invariant and one that does not, and yet all the queries the algorithm performs do not distinguish between them. The construction uses the path the algorithm takes when all Hoare queries return \(\text{false}\) as much as possible. Intuitively, such responses are less informative and rule out less transition relations, because they merely indicate the existence of a single counterexample to a Hoare triple, opposed to the result \(\text{true}\) which indicates that all transitions satisfy a property.

\begin{proof}[Proof of Thm. 6.2.]

Let \(\mathcal{A}\) be a computationally unbounded Hoare-query algorithm. We show that the number of Hoare queries performed by \(\mathcal{A}\) on transition systems from \(\mathcal{P}^{\Sigma}_{X^\perp}\) with \(|\Sigma| = n\) is at least \(2^{\frac{n+2}{2}}\). To this end, we show that if \(\mathcal{A}\) over \(|\Sigma| = 2n + 3\) performs less than \(2^n\) queries, then there exist two formulas \(\psi_1, \psi_2\) over \(y_1, \ldots, y_n, x_1, \ldots, x_n\) such that

- all the Hoare queries performed by \(\mathcal{A}\) on \(\delta^{\psi_1}_0\) and \(\delta^{\psi_2}_0\) (the transition relations of \(TS^{\psi_1}\) and \(TS^{\psi_2}\), respectively) return the same result, even though
- \(\mathcal{A}\) should return different results when run on \(TS^{\psi_1} \in \mathcal{P}^{\Sigma}_{X^\perp}\) and \(TS^{\psi_2} \in \mathcal{P}^{\Sigma}_{X^\perp}\), since \(TS^{\psi_1}\) has an invariant in Mon-CNF\(_{2n+1}\) and \(TS^{\psi_2}\) does not have an invariant (of any length).

We begin with some notation. Running on input \(TS^{\phi}\), we abbreviate \(\mathcal{H}(\delta^{\psi}_0, \cdot, \cdot)\) by \(\mathcal{H}(\cdot, \cdot, \cdot)\). Denote the queries \(\mathcal{A}\) performs and their results by \(\mathcal{H}(\phi, a_1, b_1) = b_1, \ldots, \mathcal{H}(\phi, a_m, b_m) = b_m\). We call an

\(^6\)For an arbitrary polynomial \(p(n) = \Omega(n)\), e.g., \(p(n) = c \cdot n\) with \(0 < c < 1\), enlarge \(\Sigma\), e.g., by adding to \(l_{\text{init}}\) initialization of fresh variables that are not used elsewhere, to ensure existence of an invariant of length \(\leq p(n)\).

Proc. ACM Program. Lang., Vol. 4, No. POPL, Article 5. Publication date: January 2020.
We first find a formula $\phi$ over $y_1, \ldots, y_n, x_1, \ldots, x_n$ such that the sequence of queries $A$ performs when executing on $TS^\phi$ is maximally satisfiable: if $\psi$ sat-query-agrees with $\phi$, then $\psi$ (completely) query-agrees with $\phi$ on the queries, that is,

$$\forall \psi. \ (\forall i. \ b_i = \text{false} \Rightarrow \mathcal{H}(\psi, \alpha_i, \beta_i) = b_i) \implies (\forall i. \mathcal{H}(\psi, \alpha_i, \beta_i) = b_i)$$  (3)

We construct this sequence iteratively (and define $\phi$ accordingly) by always taking $\phi$ so that the result of the next query is $\text{false}$ as long as this is possible while remaining consistent with the results of the previous queries: Initially, choose some arbitrary $\phi^0$. At each point $i$, consider the first $i$ queries $A$ performs on $\phi^i$, $\mathcal{H}(\phi^i, \alpha_i, \beta_i) = b_1, \ldots, \mathcal{H}(\phi^i, \alpha_i, \beta_i) = b_i$. If $A$ terminates without performing another query, we are done: the desired $\phi$ is $\phi_i$. Otherwise let $(\alpha_{i+1}, \beta_{i+1})$ be the next query. Amongst formulas $\phi^{i+1}$ that query-agree on the first $i$ queries, namely, $\mathcal{H}(\phi^{i+1}, \alpha_j, \beta_j) = b_j$ for all $j \leq i$, choose one such that $\mathcal{H}(\phi^{i+1}, \alpha_{i+1}, \beta_{i+1}) = \text{false}$ if possible; if such $\phi^{i+1}$ does not exist take e.g. $\phi^{i+1} = \phi^i$. The dependency of $A$ on $\phi^i$ is solely through the results of the queries to $\mathcal{H}(\delta^\phi, \cdot, \cdot)$, so $A$ performs the same $i$ initial queries when given $\phi^{i+1}$. The result is a maximally satisfiable sequence, for if a formula $\psi$ differs in query $i + 1$ in which the result is $\text{false}$ instead of $\text{true}$ we would have taken such a $\psi$ as $\phi^{i+1}$.

Let $\phi$ be such a formula with a maximally satisfiable sequence of queries $A$ performs on $\phi^i$, $\mathcal{H}(\phi, \alpha_i, \beta_i) = b_1, \ldots, \mathcal{H}(\phi, \alpha_m, \beta_m) = b_m$. For every sat $i$, take a counterexample $\sigma_i, \sigma'_i \models \alpha_i \land \delta^\phi \land \neg \beta'_i$. The single transition $(\sigma_i, \sigma'_i)$ of $S^\phi$ depends on the value of $\phi$ on at most one assignment to $\overline{x}, \overline{y}$, so there exists a valuation $v_i : \overline{y} \cup \overline{x} \rightarrow \{\text{true, false}\}$ such that

$$\forall \psi. \ (\psi(v_i) = \phi(v_i) \implies \sigma_i, \sigma'_i \models \alpha_i \land \delta^\phi \land \neg \beta'_i)$$  (4)

as well. It follows that

$$\forall \psi. \ (\psi(v_i) = \phi(v_i) \implies \mathcal{H}(\psi, \alpha_i, \beta_i) = \mathcal{H}(\phi, \alpha_i, \beta_i) = \text{false}.$$  (5)

Let $v_{i_1}, \ldots, v_{i_t}$ be the valuations derived from the sat queries (concerning indexing, $b_i = \text{false}$ iff $b_i = b_{j_i}$ for some $j$). We say that a formula $\psi$ valuation-agrees with $\phi$ on $v_{i_1}, \ldots, v_{i_t}$ if $\psi(v_{i_j}) = \phi(v_{i_j})$ for all $j$’s. Since the sequence of queries is maximally satisfiable, if $\psi$ valuation-agrees with $\phi$ on $v_{i_1}, \ldots, v_{i_t}$ then $\psi$ query-agrees with $\phi$, namely, $\mathcal{H}(\psi, \alpha_i, \beta_i) = \mathcal{H}(\phi, \alpha_i, \beta_i)$ for all $i = 1, \ldots, m$. As the dependency of $A$ on $\phi$ is solely through the results $b_1, \ldots, b_m$, it follows that $A$ performs the same queries on $\psi$ as it does on $\phi$ and returns the same answer.

It remains to argue that if $m < 2^n$ then there exist two formulas $\psi_1, \psi_2$ that valuation-agree with $\phi$ on $v_{i_1}, \ldots, v_{i_t}$ but differ in the correct result $A$ should return: $\exists \overline{y}. \forall \overline{x}. \psi_1(\overline{y}, \overline{x})$ is true, and so $TS^{\phi^i}$ has an invariant in Mon-CNF$_{2n+1}$ (Lemma 6.3), whereas $\exists \overline{y}. \forall \overline{x}. \psi_2(\overline{y}, \overline{x})$ is not, and so $TS^{\psi^i}$ does not have an invariant of any length or form (Lemma 6.3). This is possible because the number of constraints imposed by valuation-agreeing with $\phi$ on $v_{i_1}, \ldots, v_{i_t}$ is less than the number of possible valuations of $\overline{x}$ for every valuation of $\overline{y}$ and vice versa:

$$\psi_1(\overline{y}, \overline{x}) = \bigwedge_{i=1..t} \neg (\overline{y}, \overline{x}) \neq v_{i_j}$$  (6)

is true on all valuations except for some of $v_{i_1}, \ldots, v_{i_t}$, and since $t \leq m < 2^n$ there exists some $\overline{y}$ such that for all $\overline{x}$, $(\overline{y}, \overline{x})$ is not one of these valuations (recall that $|y| = n$ bits). Dually,

$$\psi_2(\overline{y}, \overline{x}) = \bigvee_{i=1..t} (\overline{y}, \overline{x}) = v_{i_j}$$  (7)
We now consider inference algorithms based on \( \mathit{itp} \). We define \( m \) with query complexity \( k \) with bounds \( (\mathsf{BMC}) \), which we formalize as follows:

\[
\forall \rho \in \mathcal{F}(\Sigma), \text{ where } \Sigma^0, \ldots, \Sigma^k \text{ are } k+1 \text{ distinct copies of the vocabulary.}
\]

We define \( \mathit{itp} \) to be the family of all interpolation-query oracles.

An algorithm in the interpolation-query model, also called an interpolation-query algorithm, is an inference from queries algorithm expecting any interpolation query oracle, where \( k_1, k_2 \) are bounded by a polynomial in \( n \) in all queries. The query complexity in this model is \( q^{\mathsf{itp}}(n) \).

Interpolation-query oracles form a family of oracles since different oracles can choose different \( \rho \) for every \( \delta, \alpha, \beta, k_1, k_2 \). Note that \( \rho \) may be exponentially long.

### 6.2 Extension to Interpolation-Based Algorithms

We now consider inference algorithms based on interpolation, another operation supported by SAT solvers. Interpolation has been introduced to invariant inference by McMillan [2003], and since extended in many works (see §3.2).

Interpolation algorithms infer invariants from facts obtained with Bounded Model Checking (BMC), which we formalize as follows:

\[
\mathcal{H}^{(k)}(\delta, \alpha, \beta) \overset{\text{def}}{=} \alpha(\Sigma^0) \land \delta(\Sigma^1) \land \ldots \land \delta(\Sigma^{k-1}, \Sigma^k) \implies \beta(\Sigma^k)
\]

for \( \alpha, \beta \in \mathcal{F}(\Sigma) \), where \( \Sigma^0, \ldots, \Sigma^k \) are \( k+1 \) distinct copies of the vocabulary.

### 6.2.1 Lower Bound on Interpolation-Query Algorithms

We show an exponential lower bound on query complexity for interpolation-query algorithms. To this end we prove the following adaptation of Thm. 6.2:

**Theorem 6.6.** Every interpolation-query inference algorithm, even computationally-unrestricted, deciding polynomial-length inference for the class of transition systems \( \mathcal{P}_{\Sigma^2}^{\mathsf{r}} \) (§6.1.1) has query complexity of \( 2^{\Omega(n)} \).

We remark that the lower bound on the interpolation-query model does not follow directly from the result for the Hoare-query model: an interpolant for \( \mathcal{H}^{(k_1+k_2)}(\delta, \alpha, \beta) = \text{true} \) depends on all traces of length \( k_1 + k_2 \) starting from states satisfying \( \alpha \), which may be an exponential number, so it cannot be computed simply by performing a polynomial number of Hoare queries to find these traces and computing an interpolant based on them. In principle, then, an interpolant can convey information beyond a polynomial number of Hoare queries. Our proof argument is therefore more subtle: we show that there exists a choice of an interpolant that is not more informative than the existence of some interpolant (i.e., only reveals information on \( \mathcal{H}^{(k_1+k_2)}(\cdot, \cdot, \cdot) \)), in the special case of systems in \( \mathcal{P}_{\Sigma^2}^{\mathsf{r}} \), in the maximally satisfiable branch of an algorithm’s execution as used in the proof of Thm. 6.2.

**Proof.** Let \( \mathcal{A} \) be a computationally unbounded algorithm using bounded reachability queries with bounds \( k_1, k_2 < r(n) \) for some polynomial \( r(n) \) (here \( n = (|\Sigma| - 1)/2 \), as in the proof of Thm. 6.2), with query complexity \( m < 2^n/r(n) \).

Proc. ACM Program. Lang., Vol. 4, No. POPL, Article 5. Publication date: January 2020.
To prove the theorem it is convenient to first consider the algorithmic model which performs bounded-reachability queries of polynomial depth but not interpolation queries, intuitively performing BMC but without obtaining interpolants from the SAT solver. Formally we consider Def. 6.4 as a query-oracle and first prove the lower bound for algorithms using this query oracle. The proof follows the argument from the proof of Thm. 6.2, relying on the fact that the BMC bounds $k_1, k_2 < r(n)$.

Assume that $A$ performs only bounded reachability queries (without obtaining interpolants). In what follows, we abbreviate $H^{(k)}(\delta^P_{\cdot, \cdot}, \cdot)$ by $H^{(k)}(\cdot, \cdot)$. We start the same as the proof of Thm. 6.2 to obtain a formula $\phi$ such that the sequence of bounded reachability queries $A$ performs when executing on $TS^\phi$ is maximally satisfiable. In this proof this reads, \[ \forall \psi. \left(\forall i. \, b_i = \text{false} \implies H^{(k)}(\phi, \alpha_i, \beta_i) = b_i\right) \implies \left(\forall i. \, H^{(k)}(\phi, \alpha_i, \beta_i) = b_i\right). \]

The main difference is that every sat query produces a counterexample trace rather than a counterexample transition as in Thm. 6.2. For every sat query $i$, we take a counterexample trace $\sigma^i_1, \ldots, \sigma^i_{k_1}$, namely, $\sigma^i_1 \models \alpha, \sigma^i_{k_1} \models \neg \beta$, and $\sigma^i_j, \sigma^i_{j+1} \models \delta^P_{\phi}$. Every such transition $\sigma^i_j, \sigma^i_{j+1} \models \delta^P_{\phi}$ depends on at most one valuation of $\phi$. Thus there exists valuations $v^i_1, \ldots, v^i_{k_1}$ so that every $\psi$ that valuation-agrees with $\phi$ on these valuations also allows the aforementioned counterexample trace, and thus $H^{(k)}(\psi, \alpha_i, \beta_i) = \text{false}$ as well. As in the proof of Thm. 6.2, it follows that if $\psi$ valuation-agrees with $\phi$ on all valuations $v^i_1, \ldots, v^i_{k_1}, \ldots, v^m_1, \ldots, v^m_m$, then all queries on $\psi$ give that same result as those on $\phi$. Since $k_1, \ldots, k_m < r(n)$, the number of these valuations is less than $r(n) \cdot m < 2^n$. The rest of the proof is exactly as in Thm. 6.2, constructing two formulas $\psi_1, \psi_2$ valuation-agreeing with $\phi$ on all valuations, but one is true (in the QBF sense) and the other is not.

We now turn to interpolation queries. Assume without loss of generality that every interpolation query is preceded by a bounded reachability query with the same bound, and that if the result is $\text{false}$ the algorithm skips the interpolation query.

Consider the algorithm’s execution on $\phi$ constructed above. We show that there exists an interpolation-query oracle that returns the same interpolants on the queries performed by the algorithm for both $\psi_1, \psi_2$ from above, and thus the algorithm’s execution still does not distinguish between them.

Consider a point when the algorithms seeks an interpolant based on $H^{(k_1+k_2)}(\phi, \alpha, \beta) = \text{true}$. Let $S$ be the set of all formulas consistent with $\phi$ on all the valuations $v_i$ from above. In particular, $H^{(k_1+k_2)}(\theta, \alpha, \beta) = \text{true}$ for all $\theta \in S$. We construct a single interpolant valid for all $\theta \in S$, that is, a formula $\rho$ s.t. for every $\theta \in S$, $H^{(k_1)}(\theta, \alpha, \rho) = \text{true}$ and $H^{(k_2)}(\theta, \rho, \beta) = \text{true}$. In particular, $\psi_1, \psi_2 \in S$, so this gives the desired interpolant for them.

Take $\hat{\delta} = \bigvee_{\theta \in S} \delta^P_{\theta}$. We argue that $H^{(k_1+k_2)}(\hat{\delta}, \alpha, \beta) = \text{true}$. For otherwise, there exists a trace $(\sigma_0, \ldots, \sigma_{k_1+k_2})$ of $\hat{\delta}$ such with $\sigma_0 \models \alpha$ and $\sigma_{k_1+k_2} \not\models \beta$. By the definition of $\hat{\delta}$, each transition $(\sigma_j, \sigma_{j+1})$ originates from $\delta^P_{\theta_j}$ for some $\theta_j \in S$. As before, this transition depends on the truth value of $\theta_j$ at one valuation $\hat{v}_j$ at the most. Furthermore, $\hat{v}_1, \ldots, \hat{v}_{k_1+k_2-1}$ are successive valuations, because all the transition systems in the class increment the valuation in the same way. Thus $\hat{v}_{j_1} \neq \hat{v}_{j_2}$. Take a formula $\hat{\theta} \in S$ that agrees with $\theta_j$ on $\hat{v}_j$ for all $j = 1, \ldots, k_1 + k_2 - 1$; one exists because

1. $\theta_j(\hat{v}_j)$ cannot contradict the valuations $\phi(v_i)$, because $\theta_j \in S$, and
2. $\theta_{j_1}(\hat{v}_{j_1})$ does not contradict $\theta_{j_2}(\hat{v}_{j_2})$ for $\hat{v}_{j_1} \neq \hat{v}_{j_2}$ for $j_1 \neq j_2$.

Thus $(\sigma_0, \ldots, \sigma_{k_1+k_2})$ is also a valid trace of $\hat{\theta} \in S$, which is a contradiction to $H^{(k_1+k_2)}(\hat{\theta}, \alpha, \beta) = \text{true}$.
Thus there exists some \( \rho \) an interpolant for \( \hat{\delta}, \alpha, \beta, k_1, k_2 \). We choose the interpolation query oracle so that
\[
Q^{(k_1,k_2)}(\theta, \alpha, \beta) = \rho
\]
for all \( \theta \in S \). This is a valid choice of interpolant: \( H^{(k_1)}(\theta, \alpha, \rho) = \text{true} \) and \( H^{(k_2)}(\rho, \beta) = \text{true} \) because \( H^{(k_1)}(\hat{\delta}, \alpha, \rho) = \text{true} \) and \( \hat{\delta} \) includes all the transitions of \( \delta_\theta^P \).

The claim follows. \( \square \)

### 6.3 Impossibility of Generalization from Partial Information

Algorithms such as PDR use generalization schemes to generalize from specific states to clauses (see §2.2 and §3.2). It is folklore that “good” generalization is the key to successful invariant inference. In this section, we apply the results of §6.1 to shed light on the question of generalization. Technically, this is a discussion of the results in §6.1.

Clearly, if the generalization procedure has full information, that is, has unrestricted access to the input—including the transition relation—then unrestricted computational power makes the problem of generalization trivial (as is every other problem!). For example, “efficient” inference can be achieved by a backward-reachability algorithm (see §2.1) that blocks counterexamples through a generalization that uses clauses from a target invariant it can compute. This setting of full-information, computationally-unrestricted generalization was used by Padon et al. [2016] in an interactive invariant inference scenario.

Our analysis in §6.1 implies that the situation is drastically different when generalization possesses partial information: the algorithm does not know the transition relation exactly, and only knows the results of a polynomial number of Hoare queries. By Thm. 6.2, no choice of generalization made on the basis on this information can in general achieve inference in a polynomial number of steps. This impossibility holds even when generalization uses unrestricted computational power, and thus it is a problem of information. To further illustrate the idea of partial information, we note that the problem remains hard even when generalization is equipped with information beyond the results of a polynomial number of Hoare queries, information of the reachability of the transition system from \( \text{Init} \) and backwards from \( \text{Bad} \) in a polynomial number of steps⁹; in contrast, information of the states reachable in any number of steps constitutes full information and the problem is again trivial with unrestricted computational power.

Finally, the same challenge of partial information is present in algorithms basing generalization on a polynomial number of interpolation queries, as follows from Thm. 6.6.

### 7 THE POWER OF HOARE-QUERIES

Hoare queries are rich in the sense that the algorithm can choose a precondition \( \alpha \) and postcondition \( \beta \) and check \( H(\delta, \alpha, \beta) \), where \( \alpha \) may be different from \( \beta \). As such, algorithms in the Hoare-query model can utilize more flexible queries beyond querying for whether a candidate is inductive. In practice, this richer form of queries facilitates an incremental construction of invariants in complex syntactic forms. For example, PDR [Bradley 2011; Eén et al. 2011] incrementally learns clauses in different frames via relative inductiveness checks, and interpolation learns at each iteration a term of the invariant from an interpolant [McMillan 2003] (see §3.2). In this section we analyze this important aspect of the Hoare-query model and show that it can be strictly stronger than inference based solely on presenting whole candidate inductive invariants. We formalize the latter approach by the model of inductiveness-query algorithms, closely related to ICE learning [Garg et al. 2014], and construct a class of transition systems for which a simple Hoare-query algorithm can infer

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⁹ This can be shown by noting that in \( \mathcal{P}_{2^P} \) (used to establish the exponential lower bound) such polynomial-reachability information can be obtained from a polynomial number of Hoare queries, reducing this scenario to the original setting.
invariants in polynomial time, but every inductiveness-query algorithm requires an exponential number of queries.

### 7.1 Inductiveness-Query Algorithms

We define a more restricted model of invariant inference using only inductiveness queries.

**Definition 7.1 (Inductiveness-Query Model).** An inductiveness-query oracle is a query oracle $Q$ such that for every $\delta$ and $\alpha \in \mathcal{F}(\Sigma)$ satisfying $Init \Rightarrow \alpha$ and $\alpha \Rightarrow \neg Bad$,

- $Q(\delta, \alpha) = true$ if $\alpha \land \delta \Rightarrow \alpha'$, and
- $Q(\delta, \alpha) = (\sigma, \sigma')$ such that $(\sigma, \sigma') \models \alpha \land \delta \land \neg \alpha'$ otherwise.

We define $I$ to be the family of all inductiveness-query oracles.

An algorithm in the inductiveness-query model, also called an inductiveness-query algorithm, is an inference from queries algorithm expecting any inductiveness query oracle. The query complexity in this model is $q^I_A(n)$.

Inductiveness-query oracles form a family of oracles since different oracles can choose different $(\sigma, \sigma')$ for every $\delta, \alpha$. Accordingly, the query complexity of inductiveness-query algorithms is measured as a worst-case query complexity over all possible choices of an inductiveness-query oracle in the family.

**ICE learning and inductiveness-queries.** The inductiveness-query model is closely related to ICE learning [Garg et al. 2014], except here the learner is provided with full information on $Init, Bad$ instead of positive and negative examples (and the algorithm refrains from querying on candidates that do not include $Init$ or do not exclude $Bad$). This model captures several interesting algorithms (see §3.2). Our complexity definition in the inductiveness-query model being the worst-case among all possible oracle responses is in line with the analysis of strong convergence in Garg et al. [2014]. Hence, lower bounds on the query complexity in the inductiveness query model imply lower bounds for the strong convergence of ICE learning. We formalize this in the following lemma, using terminology borrowed from Garg et al. [2014] (see §3.2):

**Lemma 7.2.** Let $P$ be a class of transition systems, and $L$ a class of candidate invariants. Assume that deciding the existence of an invariant in $L$, given an instance from $P$, requires at least $r$ queries in the inductiveness-query model. Then every strongly-convergent ICE-learner for $(P, L)$ has round complexity at least $r$.

**Proof.** Given a strongly-convergent ICE-learner $A$ with round-complexity at most $r$, we construct an inductiveness-query algorithm for deciding $(P, C)$ in at most $r$ queries, in the following way. Simulate at most $r$ rounds of $A$, and implement a teacher as follow: When $A$ produces a candidate $\theta \in C$,

- Check that $Init \Rightarrow \theta$, otherwise produce a positive example, a $\sigma$ s.t. $\sigma \models Init, \sigma \not\models \theta$;
- Check that $\theta \Rightarrow \neg Bad$, otherwise produce a negative example, a $\sigma$ s.t. $\sigma \models Bad, \sigma \not\models \theta$;
- Perform an inductiveness query for $\theta$. If $\theta$ is inductive, we are done—return true. Otherwise, the inductiveness-query oracle produces a counterexample—pass it to $A$.

If $r$ rounds did not produce an inductive invariant, return false.

The teacher we implement always extends the learner’s sample with an example that actually is an example in the target description (see §3.2), and that rules out the current candidate. Thus, if there exists a correct $h \in C$, $A$ finds one after at most $r$ iterations, and we return true. Otherwise, we terminate after at most $r$ with the last candidate not an inductive invariant, and we return false.

□
Inductiveness queries vs. Hoare queries. Inductiveness queries are specific instances of Hoare queries, where the precondition and postcondition are the same. Since Hoare queries can also find a counterexample in a polynomial number of queries (Lemma 5.3), inductiveness-query algorithms can be simulated by Hoare-query algorithms. Our results in the rest of this section establish that the converse is not true.

7.2 Separating Inductiveness-Queries from Hoare-Queries

In this section we show that the Hoare query model (Def. 5.2) is strictly stronger than the inductiveness query model (Def. 7.1). We will prove the following main theorem:

**Theorem 7.3.** There exists a class of systems $\mathcal{M}_E$ for which

- polynomial-length invariant inference has polynomial query complexity in the Hoare-query model (in fact, also polynomial time complexity modulo the query oracle), but
- every algorithm in the inductiveness-query model requires an exponential number of queries.

The upper bound is proved in Corollary 7.9, and the lower bound in Corollary 7.11.

7.2.1 Maximal Transition Systems for Monotone Invariants. We first define the transition systems with which we will prove Thm. 7.3. We start with a definition:

**Definition 7.4 (Maximal System).** Let $\text{Init}$, $\text{Bad}$, false and let $\varphi$ be a formula such that $\text{Init} \Rightarrow \varphi$ and $\varphi \Rightarrow \neg \text{Bad}$. The maximal transition system w.r.t. $\varphi$ is $(\text{Init}, \delta^\mathcal{M}_\varphi, \text{Bad})$ where

$$\delta^\mathcal{M}_\varphi = \varphi \rightarrow \varphi'.$$

A maximal transition system is illustrated as follows:

Note that $\delta^\mathcal{M}_\varphi$ goes from any state satisfying $\varphi$ to any state satisfying $\varphi$, and from any state satisfying $\neg \varphi$ to all states, good or bad. $\delta^\mathcal{M}_\varphi$ is maximal in the sense that it allows all transitions that do not violate the consecution of $\varphi$. Thus any transition relation $\delta$ for which $\varphi$ satisfies consecution has $\delta \Rightarrow \delta^\mathcal{M}_\varphi$.

**Lemma 7.5.** A maximal transition system $(\text{Init}, \delta^\mathcal{M}_\varphi, \text{Bad})$ has a unique inductive invariant, $\varphi$.

**Proof.** Let $I$ be any invariant of $(\text{Init}, \delta^\mathcal{M}_\varphi, \text{Bad})$. By the definition of $\delta^\mathcal{M}_\varphi$ and the fact that $\text{Init} \Rightarrow \varphi$, the set of states reachable from $\text{Init}$ is exactly the set of states satisfying $\varphi$. Thus $\varphi \Rightarrow I$.

Since $\delta^\mathcal{M}_\varphi$ allows transitions from any state satisfying $\neg \varphi$ to $\text{Bad}$, $I \Rightarrow \varphi$. □

The class of transition systems on which we focus, $\mathcal{M}_E$, is the class of maximal systems for monotone invariants, $\mathcal{M}$, together with certain unsafe systems.

Formally, for each $k \in \mathbb{N}$, we define $\mathcal{M}^k$ as the class of all transition systems $(\text{Init}_k, \delta^\mathcal{M}_\varphi, \text{Bad}_k)$ for $\text{Init}_k, \text{Bad}_k$ from $\mathcal{P}^k_{\Sigma_2}$ (§6.1.1) and $\varphi \in \text{Mon-CNF}_{2k+1}$ such that $\text{Init}_k \Rightarrow \varphi$ and $\varphi \Rightarrow \neg \text{Bad}_k$. We then define $\mathcal{M} = \bigcup_{k \in \mathbb{N}} \mathcal{M}^k$. Further, for each $k$, we take the unsafe program $E_k = (\text{Init}_k, \text{true}, \text{Bad}_k)$, and define the class $\mathcal{M}_E = \mathcal{M} \cup \{E_k \mid k \in \mathbb{N}\}$. Below we abbreviate and refer to the class $\mathcal{M}_E$ as “monotone maximal systems”.

Note that for each $k$, only a single transition system, $E_k$, in $\mathcal{M}_E$ does not have an invariant, and the others have a monotone invariant. Still, Corollary 7.11 establishes a lower bound on polynomial-length inference for $\mathcal{M}_E$ using inductiveness queries. This means that using inductiveness queries...
alone, it is hard to distinguish between monotone invariants (otherwise decision would have been feasible via search). On the other hand, with Hoare queries, search becomes feasible (establishing the upper bound).

### 7.2.2 Upper Bound for Hoare-Query Algorithms for Monotone Maximal Systems

A simple algorithm can find inductive invariants of monotone maximal systems with a polynomial number of queries. It is essentially PDR with a single frame. The ability to find invariants for $M_E$ (and check invariants) shows that it is possible to decide polynomial-length inference for $M_E$.

We now present the PDR-1 algorithm (which was also discussed in §2.2, and is cast here formally as a Hoare-query algorithm). This is a backward-reachability algorithm, operating by repeatedly checking for the existence of a counterexample to induction, and obtaining a concrete example by the method discussed in Lemma 5.3. The invariant is then strengthened by conjoining the candidate invariant with the negation of the formula $\text{Block}$. This formula is a subset of the cube of the pre-state. In PDR-1, $\text{Block}$ performs generalization by dropping a literal from the cube whenever the remaining conjunction does not hold for any state reachable in at most one step from $\text{Init}$. The result is the strongest conjunction whose negation does not exclude any state reachable in at most one step. (This might exclude reachable states in general transition systems, but not in monotone maximal systems, since maximality ensures that their diameter is one.)

**Algorithm 4**

PDR-1 invariant inference in the Hoare-query model

```plaintext
1: procedure PDR-1(Init, Bad, $[\delta]$) // Backward-reachability with PDR-1 generalization
2: $I \leftarrow \neg\text{Bad}$
3: while $\mathcal{H}(\delta, I, I) = \text{false}$ do // $I$ not inductive
4: $(\sigma, \sigma') \leftarrow \text{model}([\delta], I, \neg I')$ // counterexample to induction of $I$, implemented using Lemma 5.3
5: $d \leftarrow \text{Block-PDR-1}(\text{Init}, [\delta], \sigma)$
6: $I \leftarrow I \land \neg d$
7: return $I$
8: procedure Block-PDR-1(Init, $[\delta], \sigma$) // Generalization according to one-step reachability
9: $d \leftarrow \text{cube}(\sigma)$
10: for $l \in \text{cube}(\sigma)$ do
11: $t \leftarrow d \setminus \{l\}$
12: if $\text{Init} \implies t \land \mathcal{H}(\delta, \text{Init}, \neg t)$ then // $\text{Init} \implies t \land \text{Init} \land \delta \implies \neg t'$
13: $d \leftarrow t$
```

The main property of monotone CNF formulas we exploit in the upper bound is the ability to reconstruct them from prime consequences.

**Definition 7.6 (Prime Consequence).** A clause $c$ is a consequence of $\varphi$ if $\varphi \implies c$. A prime consequence, $c$, of $\varphi$ is a minimal consequence of $\varphi$, i.e., no proper subset of $c$ is a consequence of $\varphi$.

**Theorem 7.7 (Folklore).** If $\varphi \in \text{Mon-CNF}_n$ and a clause $c$ is a prime consequence of $\varphi$ then $c$ is a clause of $\varphi$.

Thm. 7.7 is the dual of the folklore theorem on prime implicants of monotone DNF formulas as used e.g. by Valiant [1984]. For completeness, we provide a proof here:

**Proof.** Write $\varphi = c_1 \land \ldots \land c_n$.

First we argue that $c$ is monotone. This is because dropping all positive literals from $c$ also results in a consequence $\tilde{c}$ of $\varphi$; otherwise there is a valuation $v \models \varphi, v \not\models \tilde{c}$, but $v \models c$. Consider $\tilde{v}$ which is obtained by turning the literals in $c \setminus \tilde{c}$ to false. Since $\varphi$ is monotone, $\tilde{v} \models \varphi$ still. As these literals appear positively in $c$, $\tilde{v} \not\models c$ the same way that $v \not\models \tilde{c}$. This is a contradiction to the premise.
Second, we argue that if \( c' \) is monotone and is a consequence of \( \varphi \), then there exists \( c_i \) s.t. \( c_i \subseteq c' \). Otherwise, let \( v \) be the valuation that assigns true to all variables in \( c' \) and false to the rest. Clearly \( v \not\models \varphi \). However, \( v \models c_i \) for every \( i \), since by our assumption there exists a literal \( \neg x_i \in c_i \setminus c' \) to which \( v \) assigns true. Thus \( v \models \varphi \). This is a contradiction to \( c' \) being a consequence of \( \varphi \).

The claim follows. \( \square \)

We use this property to show that PDR-1 efficiently finds the invariants of the safe maximal monotone systems \( M \), as implied by the following, slightly more general, lemma:

**Lemma 7.8.** Let \( TS = (\text{Init}, \delta, \text{Bad}) \) be a transition system over \( \Sigma \), \( n = |\Sigma| \), and \( m \in \mathbb{N} \) such that

(i) \( TS \) is safe,
(ii) every reachable state in \( TS \) is reachable in at most one step from \( \text{Init} \),
(iii) this set can be described by a Mon-CNF formula, namely, there is \( \varphi \in \text{Mon-CNF}_m \) such that

\[
\sigma \models \varphi \iff \sigma \models \text{Init} \lor \exists \sigma_0 \in \text{Init} \text{ s.t. } (\sigma_0, \sigma) \models \delta.
\]

Then PDR-1(Init, Bad, [\delta]) returns the inductive invariant \( \varphi \) for TS with at most \( n \cdot m \) Hoare queries.

**Proof.** Let \( \varphi \) be as in the premise. We show that \( I \) of Alg. 4 (1) always overapproximates \( \varphi \), (2) is strengthened with a new clause from \( \varphi \) in every iteration.

(1) We claim by induction on the number of iterations in Alg. 4 that \( \varphi \implies I \). Clearly this holds initially. In line 4, \( \sigma \not\models \varphi \), otherwise \( \sigma' \models \varphi \), and \( \varphi \implies I \) gives \( \sigma' \models I \) which is a contradiction to \( (\sigma, \sigma') \) being a CTI. Now, for every \( \sigma \not\models \varphi \), its minimization \( \neg d \) is a consequence of \( \varphi \), namely, \( \varphi \implies \neg d \), because \( \neg d \) holds for all states reachable in at most one step (\( \text{Init} \implies \neg d \), \( \text{Init} \land \delta \implies \neg d' \)) and those are states satisfying \( \varphi \). Thus also \( \varphi \implies I \land \neg d \).

(2) As we have argued earlier, \( \neg d \) in line 5 is a consequence of \( \varphi \). We refer to it as the clause \( c = \neg d \). We argue that \( c \) is a clause of \( \varphi \). By Thm. 7.7 is suffices to show that \( c \) is a prime consequence of \( \varphi \), seeing that \( \varphi \) is monotone. Assume (for the sake of contradiction) that \( \tilde{c} \subsetneq c \) is a consequence of \( \varphi \). Consider the minimization procedure as it attempts to remove a literal \( \tilde{l} = (\neg c) \setminus (\neg \tilde{c}) \) (line 11). This literal is not removed, so \( \text{Init} \land t \) or \( \text{Init} \land \delta \land t' \) is satisfiable at this point. So there is a state reachable in at most one step that satisfies \( t \), which means that \( \varphi \land t \) is satisfiable. From this point onwards, literals are only omitted from \( t \), apart from \( \tilde{l} \) that is resurrected; thus \( \neg c \subseteq t \cup \{\tilde{l}\} \). These are conjunctions, so \( \varphi \land (\neg c \setminus \{\tilde{l}\}) \) is satisfiable. But this means that \( \varphi \not\models (c \setminus \{\tilde{l}\}) \). In particular, it follows that \( \varphi \not\models \tilde{c} \) since \( \tilde{c} \subseteq c \setminus \{\tilde{l}\} \). Thus \( \tilde{c} \) is not a consequence of \( \varphi \), which is a contradiction to the premise. Therefore \( c \) must be a prime consequence of \( \varphi \).

It remains to argue that \( s \) in line 5 is not already present in \( I \). But this is true because \( \sigma \models s \), and \( s \not\models I \).

Overall, after at most \( m \) such iterations, \( I \implies \varphi \) from (2), and also \( \varphi \implies I \) from (1). Thus \( I \equiv \varphi \), which is indeed an inductive invariant (it captures exactly the reachable states). Minimization performs \( n = |\Sigma| \) queries, and so the total number of queries is at most \( nm \). \( \square \)

From this lemma and the uniqueness of the invariants (Lemma 7.5) the upper bound for \( M_E \) follows easily:

**Corollary 7.9.** Polynomial-length invariant inference of \( M_E \) can be decided in a polynomial number of Hoare queries.

**Proof.** Let \( p(\cdot) \) be the polynomial dictating the target length in Def. 4.1. The Hoare-query algorithm runs PDR-1 for \( p(n) \cdot n \) queries. If PDR-1 does not terminate, return no. Otherwise, it produces a candidate invariant \( \psi \). If \( \psi \not\models \text{CNF}_{p(n)} \) return no. Perform another check for whether \( \psi \) is indeed inductive: if it is inductive, return yes, otherwise no.

Proc. ACM Program. Lang., Vol. 4, No. POPL, Article 5. Publication date: January 2020.
Correctness: let \((\text{Init}, \delta, \text{Bad}) \in \mathcal{M}_E\). If there exists an inductive invariant in \(\text{CNF}_{p(n)}\), it is unique, and is the formula \(\varphi \in \text{Mon-CNF}_{p(n)}\) that characterizes the set of states reachable in at most one step. By Lemma 7.8 PDR-1 finds \(\varphi\) in a polynomial number of Hoare queries. Otherwise, \((\text{Init}, \delta, \text{Bad})\) is not safe, or its unique inductive invariant \(\varphi \notin \text{CNF}_{p(n)}\). In both cases PDR-1 cannot produce an inductive invariant in \(\text{CNF}_{p(n)}\), and terminates/is prematurely terminated after \(p(n) \cdot n\) Hoare queries.

**Remark 7.1.** The condition that the invariant is monotone in Lemma 7.8 can be relaxed to pseudomonotonicity: A formula \(\varphi\) in CNF is pseudo-monotone if no propositional variable appears in \(\varphi\) both positively and negatively. Thus it can be made monotone by renaming variables. It still holds for a pseudo-monotone CNF \(\varphi\) that a prime consequence is a clause of \(\varphi\), and therefore PDR-1 successfully finds an invariant in a polynomial number of Hoare queries also for the class of maximal systems for pseudo-monotone invariants.

### 7.2.3 Lower Bound for Inductiveness-Query Algorithms for Monotone Maximal Systems

We now prove that every inductiveness-query algorithm for the class of monotone maximal systems requires exponential query complexity. The main idea of the proof is that inductiveness-query algorithms are oblivious to adding transitions:

**Theorem 7.10.** Let \(X, Y\) be sets of transition systems, such that \(Y\) covers the transition relations of \(X\), that is, for every \((\text{Init}, \delta, \text{Bad}) \in X\) there exists \((\text{Init}, \hat{\delta}, \text{Bad}) \in Y\) over the same vocabulary s.t.

1. \(\delta \implies \hat{\delta}\), and
2. if \((\text{Init}, \delta, \text{Bad})\) has an inductive invariant in \(\text{CNF}_{p(n)}\), then so does \((\text{Init}, \hat{\delta}, \text{Bad})\).

Then if \(\mathcal{A}\) is an inductiveness-query algorithm for \(Y\) with query complexity \(t\), then \(\mathcal{A}\) is also an inductiveness-query algorithm for \(X\) with query complexity \(t\).

**Proof.** Let \(\mathcal{A}\) be an algorithm for \(Y\) as in the premise. We show that \(\mathcal{A}\) also solves the problem for \(X\). Let \((\text{Init}, \delta, \text{Bad}) \in X\) and analyze \(\mathcal{A}^Q(\text{Init}, \delta, [\delta])\), where \(Q\) is some inductiveness-query oracle. Consider the first \(t\) candidates, \(\alpha_1, \ldots, \alpha_t\). If one of them is an inductive invariant for \((\text{Init}, \delta, \text{Bad})\), we are done (recall that the inductiveness query is only defined for queries with \(\alpha_i\) s.t. \(\text{Init} \Rightarrow \alpha_i\) and \(\alpha_i \Rightarrow \neg \text{Bad}\)). If we are not done, let \((\text{Init}, \hat{\delta}, \text{Bad}) \in Y\) as in the premise for the given \((\text{Init}, \delta, \text{Bad})\). We show that in this case \(\mathcal{A}^Q(\text{Init}, \hat{\delta}, [\hat{\delta}])\) simulates \(\mathcal{A}^Q(\text{Init}, \delta, [\delta])\) where \(Q'\) is an inductiveness-query oracle derived from \(Q\) by \(Q'(\delta, \alpha_i) = Q(\delta, \alpha_i)\) for all \(i = 1, \ldots, t\). Note that \(Q'(\hat{\delta}, \cdot)\) is a valid inductiveness-query oracle: by the assumption that \(\alpha_i\) is not inductive for \(\delta, Q(\delta, \alpha) = (\sigma, \sigma')\), that is, \(\sigma, \sigma' \models \alpha \land \delta \lor \neg \alpha'\). From condition 1, \(\delta \implies \hat{\delta}\), and so we deduce that also \(\sigma, \sigma' \models \alpha \lor \hat{\delta} \land \neg \alpha'\). Therefore, after at most \(t\) queries, \(\mathcal{A}^Q(\text{Init}, \hat{\delta}, [\hat{\delta}])\) terminates, returning either (i) an inductive invariant \(\varphi \in \text{CNF}_{p(n)}\) for \((\text{Init}, \hat{\delta}, \text{Bad})\), which is also an inductive invariant for \((\text{Init}, \delta, \text{Bad})\), by condition 1; or (ii) no inductive invariant in \(\text{CNF}_{p(n)}\) for \((\text{Init}, \hat{\delta}, \text{Bad})\), in which case this is also true for \((\text{Init}, \delta, \text{Bad})\), by condition 2. Either way \(\mathcal{A}^Q(\text{Init}, \delta, [\delta])\) is correct and uses \(\leq t\) queries.

The lower bound for monotone maximal systems results from Thm. 7.10 together with the hardness previously obtained in Thm. 6.2.

**Corollary 7.11.** Every inductiveness-query algorithm, even computationally-unrestricted, deciding polynomial-length inference for \(\mathcal{M}_E\) has query complexity of \(2^{\Omega(n)}\).

**Proof.** For \(\mathcal{P}_{2^F}\) with invariant class \(\text{Mon-CNF}_n\), an exponential number of Hoare queries is necessary, by Thm. 6.2. It follows that in the inductiveness-query model, an exponential query
Table 1. Concept vs. invariant learning: query complexity of learning Mon-CNF\(_n\)

| Invariant Inference | Concept Learning |
|---------------------|------------------|
| Maximal Systems     | General Systems  |
| Inductiveness       | Exponential      |
|                     | (Corollary 7.11) |
|                     | Exponential      |
|                     | (Thm. 6.2)       |
| Hoare              | Polynomial       |
|                     | (Corollary 7.9)  |
|                     | Exponential      |
|                     | (Thm. 6.2)       |
|                     | Equivalence      |
|                     | Polynomial       |
|                     | [Angluin 1987; Hellerstein et al. 2012] |
|                     | Subexponential\(^1\) / Polynomial\(^2\) |

\(^1\) proper learning
\(^2\) with exponentially long candidates

complexity is also required (since a Hoare-query algorithm can implement a valid inductiveness-query oracle). By arguing that \( \mathcal{M}_E \) covers \( \mathcal{P}_{\Sigma^P} \) we can apply Thm. 7.10 to deduce that \( \mathcal{M}_E \) with invariant class Mon-CNF\(_n\) also necessitates an exponential number of inductiveness queries:

Let \((\text{Init}_k, \delta, \text{Bad}_k) \in \mathcal{P}_{\Sigma^P}\). Recall that in these systems, \( n = 2k + 3 \) (the vocabulary size). If the system does not have an inductive invariant in Mon-CNF\(_n\), then \( E_k = (\text{Init}_k, \text{true}, \text{Bad}_k) \in \mathcal{M}_E \) satisfies the conditions of Thm. 7.10 (condition 1 holds as evidently \( \delta \implies \text{true} \), and condition 2 holds vacuously). Otherwise, there exists an inductive invariant \( \varphi \in \text{Mon-CNF}\(_n\) \) for \((\text{Init}_k, \delta, \text{Bad}_k)\). In this case, the system \((\text{Init}_k, \delta^M, \text{Bad}_k)\) satisfies the conditions of Thm. 7.10: condition 1 is due to the maximality of \( \delta^M \), and 2 holds as \( \varphi \) is an inductive invariant.

Thus \( \mathcal{M}_E \) with the class Mon-CNF\(_n\) requires an exponential number of inductiveness queries. Since \( \mathcal{M}_E \) has a monotone invariant or none at all, it follows that an exponential number inductiveness queries is also required for \( \mathcal{M}_E \) with CNF\(_n\), as desired.

We note that the transition relations in \( \mathcal{M}_E \) are themselves polynomial in \( |\Sigma| \). Hence the query complexity in this lower bound is exponential not only in \( |\Sigma| \) but also in \( |\delta| \) (see Remark 5.2).

Finally, it is interesting to notice that the safe systems in \( \mathcal{M}_E \) have a unique inductive invariant, and still the problem is hard.

8 INVARIANT LEARNING & CONCEPT LEARNING WITH QUERIES

The theory of exact concept learning [Angluin 1987] asks a learner to identify an unknown formula\(^{10}\) \( \varphi \) from a class \( \mathcal{L} \) using queries posed to a teacher. Prominent types of queries include membership—given state \( \sigma \), return whether \( \sigma \models \varphi \)—and equivalence—given \( \theta \), return true if \( \theta \equiv \varphi \) or, otherwise, a counterexample, a \( \sigma \) s.t. \( \sigma \not\models \theta \), \( \sigma \models \varphi \) or vice versa.

What are the connections and differences between concept learning formulas in \( \mathcal{L} \) and learning invariants in \( \mathcal{L} \)? Can concept learning algorithms be translated to inference algorithms? These questions have spurred much research [e.g. Garg et al. 2014; Jha and Seshia 2017]. In this section we study these questions with the tool of query complexity and our aforementioned results.

The most significant outcome of this analysis is a new hardness result (Corollary 8.1) showing that ICE-learning is provably harder than classical learning: namely, that, as advocated by Garg et al. [2014], learning from counterexamples to induction is inherently harder than learning from examples labeled positive or negative. The proof of this result builds on the lower bound of Corollary 7.11. We also establish (im)possibility results for directly applying algorithms from concept learning to invariant inference.

Complexity: the easy, the complex, and the even-more-complex. In this paper we have studied the complexity of inferring \( \mathcal{L} = \text{Mon-CNF}\(_n\) \) invariants using Hoare/inductiveness queries in two settings: for general systems (in §6.1), and for maximal systems in §7. Table 1 summarizes our results

\(^{10}\)In general, a concept is a set of elements; here we focus on logical concepts.
and contrasts them with known complexity results in classical concept learning for the same class of formulas. For the sake of the comparison, the table maps inductiveness queries to equivalence queries (as these are similar at first sight) and maps the more powerful setting of Hoare queries to the more powerful setting of equivalence and membership queries.

Starting with similarity, the gap in the complexity between Hoare- and inductiveness-queries in learning invariants for maximal systems parallels the gap between equivalence and equivalence + membership queries in concept learning. Our proof for the upper bound for Hoare queries is related to the upper bound in concept learning and simulations of concept learning algorithms (see below), but the lower bound for inductiveness queries uses very different ideas, and establishes stronger lower bounds than possible in concept learning, as we describe below.

The similarity ends here. First, general systems are harder, and inferring \( \mathcal{L} = \text{Mon-CNF}_n \) invariants for them is harder than concept learning with the same \( \mathcal{L} \), even with the full power of Hoare queries. This, unsurprisingly, illustrates the challenges stemming from transition systems with complex reachability patterns, such as a large diameter. Second, even the hard cases for concept learning have lower complexity than the hard invariant inference problems: learning concepts in \( \mathcal{L} = \text{Mon-CNF}_n \) has subexponential query complexity (or even polynomial complexity when exponentially-long candidates are allowed), whereas we prove exponential lower bounds for inference. One important instance of this discrepancy shows that inductiveness queries are inherently weaker than equivalence queries, as learning Mon-CNF \( _n \) invariants in the inductiveness model is harder than learning Mon-CNF \( _n \) formulas using equivalence queries. Put differently, this is a hardness result for concept learning with \textit{ICE-equivalence queries}, which are like equivalence queries, only when the given \( \theta \) is not equivalent to the target concept \( \phi \) the teacher responds with an implication counterexample [Garg et al. 2014]: a pair \( \sigma, \sigma' \) s.t. \( \sigma \models \theta \) and \( \sigma' \not\models \theta \), but \( \sigma \not\models \phi \) or \( \sigma' \models \phi \). Our results thus imply:

\[ \text{Corollary 8.1. There exists a class of formulas } \mathcal{L} \text{ that can be learned using a subexponential number of equivalence queries, but requires an exponential number of ICE-equivalence queries.} \]

This result quantitatively corroborates the difference between counterexamples to induction and examples labeled positive or negative, a distinction advocated by Garg et al. [2014].

The higher complexity of inferring invariants has consequences for the feasibility of simulating queries (and algorithms) from concept learning in invariant inference, as we discuss next.

### Queries: some unimplementable algorithms

Table 2 summarizes our results for the possibility and impossibility of simulating concept learning algorithms in invariant learning. This table depicts implementability (✓) or unimplementability (✗) of membership and equivalence queries used in concept learning a class of formulas \( \mathcal{L} \) through inductiveness and Hoare queries used in learning invariants for maximal systems over \( \mathcal{L} \), and for general systems with candidate invariants in \( \mathcal{L} \). The proofs of impossibilities are based on the differences in complexity described above: that neither equivalence nor membership queries can be simulated over general systems using even Hoare queries is implied by the hardness of general systems; that neither equivalence nor membership can be simulated even over maximal systems using inductiveness queries is implied by the higher complexity of these compared to concept learning. The only possibility result is of simulating

### Table 2. Concept vs. invariant learning: implementability of concept-learning queries

|                         | Maximal Systems | General Systems |
|-------------------------|-----------------|-----------------|
| **Inductiveness**       |                 |                 |
| **Hoare**               | ✓               | ✓               |
| **Equivalence**         | ✗               | ✗               |
| **Membership**          | ✗               | ✗               |

Proc. ACM Program. Lang., Vol. 4, No. POPL, Article 5. Publication date: January 2020.
inductiveness and membership queries using Hoare queries over maximal systems; the idea is that a Hoare query $H(\delta_\phi^M, \text{Init}, \neg\text{cube}(\sigma)) \not\models \text{false}$ implements a membership query on $\sigma$, thanks to fact that the inductive invariant is exactly the set of states reachable in one step, and that a membership query can disambiguate a counterexample to induction into a labeled example, so it is possible to simulate an equivalence query by an inductiveness query. Interestingly, the algorithm we use to show the polynomial upper bound on Hoare queries for maximal systems, PDR-1, can be obtained as such a translation of an algorithm from Angluin [1987] performing concept learning of Mon-CNF$_n$ using equivalence and membership queries.

9 RELATED WORK

Complexity of invariant inference. The fundamental question of the complexity of invariant inference in propositional logic has been studied by Lahiri and Qadeer [2009]. They show that deciding whether an invariant exists is PSPACE-complete. This includes systems with only exponentially-long invariants, which are inherently beyond reach for algorithms aiming to construct an invariant. In this paper we focus on the search for polynomially-long invariants. Lahiri and Qadeer [2009] study the related problem of template-based inference, and show it is $\Sigma^p_2$-complete. Polynomial-length inference for CNF formulas can be encoded as specific instances of template-based inference; the $\Sigma^p_2$-hardness proof of Lahiri and Qadeer [2009] uses more general templates and therefore does not directly imply the same hardness for polynomial-length inference. The same work also shows that inference is only $\Pi^p_1 = \text{coNP}$-complete when candidates are only conjunctions (or, dually, disjunctions). In this paper we focus on the richer class of CNF invariants.

Black-box invariant inference. Black-box access to the program in its analysis is widespread in research on testing [e.g. Nidhra and Dondeti 2012]. In invariant inference, Daikon [Ernst et al. 2001] initiated the black-box learning of likely program invariants [see e.g. Csallner et al. 2008; Sankaranarayanan et al. 2008]. In this paper we are interested in inferring necessarily correct inductive invariants. The ICE learning model, introduced by Garg et al. [2014, 2016], and extended to general Constrained Horn Clauses in later work [Ezudheen et al. 2018], pioneered a black-box view of inference algorithms such as Houdini [Flanagan and Leino 2001] and symbolic abstraction [Reps et al. 2004; Thakur et al. 2015]. The inductiveness model in our work is inspired by this work, focusing on black-box access to the transition relation while providing the learner with full knowledge of the set of initial and bad states. Capturing PDR in a black-box model was achieved by extending ICE with relative-inductiveness queries [Vizel et al. 2017]. Our work shows that an extension is necessary, and applies to any Hoare-query algorithm.

Lower bounds for black-box inference. To the best of our knowledge, our work provides the first unconditional exponential lower bound for rich black-box inference models such as the Hoare-query model. An impossibility result for ICE learning in polynomial time in the setting of quantified invariants was obtained by Garg et al. [2014], based on the lower bound of Angluin [1990] for concept learning DFAs with equivalence queries. Our lower bound for monotone maximal systems (i) demonstrates an exponential gap between ICE learning and Hoare-query algorithms such as PDR (§7), and (ii) separates ICE learning from concept learning (§8); in particular, it holds even when candidates may be exponentially long (see Corollary 7.11 and Garg et al. [2013, Appendix B]).

Learning and synthesis with queries. Connections with exact learning with queries [Angluin 1987] are discussed in §8. The lens of synthesis has inspired many works applying ideas from machine learning to invariant inference [e.g. Garg et al. 2014; Jha et al. 2010; Sharma and Aiken 2016; Sharma et al. 2013b,a, 2012]. The role of learning with queries is recognized in prominent synthesis approaches such as Counterexample-Guided Inductive Synthesis (CEGIS) [Solar-Lezama et al. 2006] and synthesizer-driven approaches [e.g. Gulwani 2012; Jha et al. 2010; Le et al. 2017], which learn...
from equivalence and membership queries [Alur et al. 2015; Bshouty et al. 2017; Drachsl-Cohen et al. 2017; Jha and Seshia 2017]. The theory of oracle-guided inductive synthesis [Jha and Seshia 2017] theoretically studies the convergence of CEGIS in infinite concept classes using different types of counterexamples-oracles, and relates the finite case to the teaching dimension [Goldman and Kearns 1995]. In this work we study inference based on a different form of queries, and prove lower bounds on the convergence rate in finite classes.

**Proof complexity.** Proof complexity studies the power of polynomially-long proofs in different proof systems. A seminal result is that a propositional encoding of the pigeonhole principle has no polynomial resolution proofs [Haken 1985]. Ideas and tools from proof complexity have been applied to study SAT solvers [e.g. Pipatsrisawat and Darwiche 2011] and recently also SMT [Robere et al. 2018]. Proof complexity is an alternative technical approach to study the complexity of proof search algorithms, by showing that some instances do not have a short proof, showing a lower bound regardless of how search is conducted. Our work, inspired by learning theory, provides exponential lower bounds on query-based search even when the proof system is sufficiently strong to admit short proofs: in our setting, there is always a short derivation of an inductive invariant by generalization in backward-reachability, blocking counterexamples with the optimal choice, using clauses from a target invariant (see §6.3). We expect that proof complexity methods would prove valuable in further study of inference.

10 CONCLUSION

Motivated by the rise of SAT-based invariant inference algorithms, we have attempted to elucidate some of the principles on which they are based by a theoretical complexity analysis of algorithms attempting to infer invariants of polynomial size. We have developed information-based analysis tools, inspired by machine learning theory, to investigate two focal points in SAT-based inference design: (1) **Generalization**, which we have shown to be impossible from a polynomial number of Hoare queries in the general case; (2) **Rich Hoare queries**, beyond presenting candidate invariants, which we have shown to be pivotal in some cases. Our upper bound for PDR on the class of monotone maximal systems is a first step towards theoretical conditions guaranteeing polynomial running time for such algorithms. One lesson from our results is the importance of characteristics of the transition relations (rather than of candidate invariants), which make the difference between the lower bound for general systems (Thm. 6.2) and the upper bound for maximal systems (Corollary 7.9), both for the same class of candidate invariants. We believe that theoretical guarantees of efficient inference would involve special classes of transitions systems and algorithms using repeated generalization employing rich Hoare queries.

At the heart of our analysis lies the observation that many interesting SAT-based algorithms can be cast in a black-box model. This work focuses on the limits and opportunities in black-box inference and shows interesting information-theoretic lower bounds. One avenue for further research is an information-based analysis of black-box models extended with white-box capabilities, e.g. by investigating syntactical conditions on the transition relation that simplify generalization.

ACKNOWLEDGMENTS

We thank our shepherd and the anonymous referees for comments that improved the paper. We thank Kalev Alpernas, Nikolaj Bjørner, P. Madhusudan, Yishay Mansour, Oded Padon, Hila Peleg, Muli Safra, and James R. Wilcox for insightful discussions and suggestions, and Gil Buchbinder for saving a day. The research leading to these results has received funding from the European Research Council under the European Union’s Horizon 2020 research and innovation programme (grant agreement No [759102-SVIS]). This research was partially supported by the National Science Foundation (NSF) grant no. CCF-1617498, by Len Blavatnik and the Blavatnik Family foundation,
the Blavatnik Interdisciplinary Cyber Research Center, Tel Aviv University, the United States-Israel Binational Science Foundation (BSF) grant No. 2016260, and the Israeli Science Foundation (ISF) grant No. 1810/18.
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Proc. ACM Program. Lang., Vol. 4, No. POPL, Article 5. Publication date: January 2020.
A DUALITY OF BACKWARD- & FORWARD-REACHABILITY

Throughout the paper we study invariant inference w.r.t. CNF formulas with $p(n)$ clauses (where $n = |\Sigma|$). Our results apply also to the case of Disjunctive Normal Form (DNF) formulas with at most $p(n)$ cubes. This is a corollary of the known duality between backward- and forward-reachability:

The dual transition system is $(\text{Init}, \delta, \text{Bad})^* \overset{\text{def}}{=} (\text{Bad}, \delta^{-1}, \text{Init})$ where $\delta^{-1}$ is the inverse (between pre- and post-states) of the transition relation, obtained from $\delta$ by switching the roles of $\Sigma$ and $\Sigma'$. The dual of a class of transition systems is the class of dual transition systems. The dual of a formula is $\varphi^* \overset{\text{def}}{=} \neg \varphi$. The dual of a class of formulas is the class of dual formulas. We have that $I$ is an inductive invariant w.r.t. $(\text{Init}, \delta, \text{Bad})$ iff $I^*$ is an inductive invariant w.r.t. $(\text{Init}, \delta, \text{Bad})^*$. For an algorithm $\mathcal{A}$, The dual algorithm $\mathcal{A}^*$ is the algorithm that, given as input $(\text{Init}, \delta, \text{Bad})$, executes $\mathcal{A}$ on $(\text{Init}, \delta, \text{Bad})^*$ and returns the dual invariant. By applying the dual algorithm to the dual transition systems and target invariants, we obtain:

**Lemma A.1.** Polynomial-length inference of $\mathcal{P}$ w.r.t. CNF$_{p(n)}$ has the same complexity as polynomial-length inference of $\mathcal{P}^*$ w.r.t. DNF$_{p(n)}$.

B POLYNOMIAL-LENGTH TRANSITION SYSTEMS AND HOARE INFORMATION COMPLEXITY

In our definitions, the complexity of a black-box query-based inference algorithm (Def. 5.4) is a function of the target invariant length derived from the vocabulary size, and does not depend on the length of the representation of the transition relation, which the inference algorithm cannot access directly. Accordingly, the general case in our lower bound on the query complexity of Hoare-query algorithms is the class of all transition systems, and we show that to solve the general case the number of Hoare queries must be exponential in $n = |\Sigma|$. We emphasize that this result holds despite the reasonably-sized class of target invariants (an exponential number, not doubly exponential), and that Hoare queries are rich (can be used with any precondition and postcondition).

Can inference algorithms utilize an assumption that the transition relation can be expressed by formulas of polynomial size? Formally, this asks for an analysis of the query complexity as it depends also on $|\delta|$ in addition to $|\Sigma|$. An important technical difference is that in this setting an algorithm may attempt to “breach” our black-box definition, and (concept-) learn the transition relation formula itself; once it is obtained the algorithm can deduce from it whether an invariant exists using unlimited computational power (see §6.3). The possibility of such concept learning reflects on the statement of Thm. 6.1 when the complexity definition is altered. With unlimited computational power and exponentially-long queries, the algorithm can learn the formula of $\delta$:

**Lemma B.1.** There exists a computationally unrestricted Hoare-query inference algorithm $\mathcal{A}^H$ with query complexity polynomial in $|\Sigma|$, $|TS|$ for the class of transition systems $\mathcal{P}_{\Sigma^2}$ (§6.1.1).

**Proof.** Assume we are attempting to infer with Hoare queries an invariant for $TS^\phi \in \mathcal{P}^k_{\Sigma^2}$, with $|\phi| \leq m$. We show how to identify $\phi$ in a number of Hoare queries polynomial in $m$, from which using unlimited computational power the algorithm can check if an invariant for $TS^\phi$ exists.

Use the halving algorithm/majority vote [Angluin 1987; Barzdins and Freivald 1972; Littlestone 1987] to learn $\phi$. For completeness, we describe it here: At each step, consider $S$, the set of formulas (over the same vocabulary as $\phi$) of length at most $m$ that are consistent with the results of the queries performed so far (namely, $\theta \in S$ if performing the same Hoare queries on $TS^\phi$ yields the same results as were observed). We can terminate if $S$ includes only one formula. Otherwise, take $\hat{\phi} \in S$ to be the formula that is true on a valuation $v$ iff the majority of formulas in $S$ so far are true on $v$. Check whether $\phi \equiv \hat{\phi}$ using a Hoare query to be described below. If $\phi \equiv \hat{\phi}$ we are done,
otherwise we obtain a counterexample: a valuation on which ϕ, ˆϕ disagree. In the next step, the set S is reduced by at least a factor of two, so the process terminates after a number of iterations polynomial in m.

It remains to implement using Hoare queries the check of whether ϕ ≡ ˆϕ and obtaining a counterexample. This can be done using the query H(ϕ, α, β) where: α is the formula ¬a ∧ ¬b ∧ ¬e (with any ⃗y, ⃗x), and β is the post-image of TS ˆϕ on α. If the result is true, the equivalence query returns true. Otherwise, the valuation differentiating ϕ, ˆϕ is obtained from the pre-state (in the propositions ⃗y, ⃗x) of the counterexample to the Hoare query (using Lemma 5.3). This is correct because δPϕ, δP ˆϕ have different transitions from the same state σ iff ϕ(⃗y, x) = ˆϕ(⃗y, x) where (⃗y, ⃗x) are from the interpretation of these propositions in σ. □

As Angluin [1987] recognizes, this result relies on queries on candidates that are exponentially-long. When queries can be performed only on polynomially-long formulas and their choice can use unrestricted computational power, the question of whether a result analogous to Thm. 6.2 exists is related to open questions in concept learning, such as whether a polynomial number of equivalence and membership queries can identify a formula of length at most m [Bshouty et al. 1996]. We thus propose the following conjecture, a variant of Thm. 6.2 where the complexity depends also on the size of the transition relation:

**Conjecture B.2.** Every Hoare-query inference algorithm A^H, even computationally-unrestricted, querying on formulas polynomial in |Σ| + |TS|, for the class of transition systems PΣ^T (§6.1.1) and and for any class of target invariants L s.t. Mon-CNFn ⊆ L, has query complexity superpolynomial in |Σ| + |TS|.

If Conjecture B.2 is true, a result analogous to Thm. 6.1 can be obtained, obtaining superpolynomial lower bounds not only in |Σ| but also in |TS|.

We emphasize that the exponential lower bound we obtain in Thm. 7.3 is already exponential also in |TS| (and this holds even when candidates can be exponentially long), as the transition relations in ME are all of size polynomial in their vocabulary.

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11 Corollary 7.11 implies that inductiveness queries alone cannot perform this check, because there the transition relation formulas are also polynomial in n, as we discuss below concerning the results of Thm. 7.3.