Learning Models from Temporal-Logic Properties via Explanations

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Abstract

Given a model and a property expressed in temporal logic, a model checker normally produces a counterexample in case the model does not satisfy the property. This counterexample is meant to serve as a guide for manually modifying the model so that the new model does satisfy the property. We observe that basing the modification of a model on negative information (why a formula is not true) can have limitations, and we present a method employing positive information instead. Our method incrementally learns a subformula and marks the part of the model that makes the already learned subformula true (i.e. an *explanation*). Next, our method attempts to learn the rest of the formula without altering the marked part of the model.

Introduction

Model checking (Clarke, Grumberg, & Peled 1999) is a collection of techniques for verifying properties of systems having an ongoing interaction with the environment. A model checker has as input a model representing a system and a temporal-logic formula expressing a desirable property. The output is either a confirmation or a denial that the property holds. In case of denial, the model checker normally produces a *counterexample*, consisting of a part of the model that makes the formula false. This counterexample is intended as a guide for manually modifying the model so that the violated property is satisfied. Our objective will be to study a method for automatically modifying a faulty model using *explanations* instead of counterexamples.

Industry has increasingly been using model-checking methods for at least two reasons. First, model checking can often detect faults eluding more traditional methods such as testing. Second, state-of-the-art implementations of model checkers, employing binary decision diagrams (Bryant 1992), allow the verification of properties in systems with many states. Model checking has thus found numerous applications, such as verifying digital circuits, developing critical software, and more recently exploring biological systems.

One of the most appreciated features of model checkers is their ability to generate a counterexample if the model does not satisfy a given property. Such a counterexample is a path that demonstrates why the formula representing such a property does not hold in the model. Hence, to make the formula hold true, we must modify at least the part of the model generating such a path. Once modified, we can ask the model checker again if the new model satisfies the property.

We are interested in mechanizing this transformation process of the given model. Of the many temporal logics used in model checking, we selected "computation-tree logic" (CTL) (Clarke, Grumberg, & Peled 1999), because of its simple model-checking algorithm compared with that of other logics. Moreover, motivated by some practical applications (Espinosa-Soto, Padilla-Longoria, & Alvarez-Buylla 2004), we limit ourselves to models having the same set of states as that of the faulty, given model.

Computation-Tree Logic

Definition 1. *Given a finite set* Prop *of* propositional variables*, a* Kripke structure *or* model $\mathcal{M} = \langle S, R, L\rangle$ *consists of a finite set* S *of* states*, a total relation* $R \subseteq S^2$ *over* S *(i.e. for every* $s \in S$ *there exists* $t \in S$ *such that* $(s,t) \in R$*), called the* accessibility relation*, and a* labelling function $L : S \to 2^{\mathrm{Prop}}$.

Kripke structures are often represented graphically as illustrated by $\mathcal{M}_0 = \langle\{s_0, s_1\}, \{(s_0, s_1), (s_1, s_1)\}, \{(s_0, \emptyset), (s_1, \{p\})\}\rangle$:

Definition 2. *A* path *of* $\mathcal{M}$ *is an infinite sequence* $s_0, s_1, \ldots$ *of states* $s_i \in S$*, such that for all* $i \in \mathbb{N}$*,* $(s_i, s_{i+1}) \in R$.

Throughout, $\mathcal{M}$ denotes Kripke structures, S sets of states, R accessibility relations, L labelling functions, p, q, and r propositional variables, and s and t states. In addition, Greek letters denote formulas.

Definition 3. Basic Computation-tree logic (**CTL**) *formulas have the following syntax given in BNF:*

$$\alpha ::= \top \,|\, p \,|\, (\neg\alpha) \,|\, (\alpha \wedge \alpha) \,|\, (\mathbf{EX}\,\alpha) \,|\, (\mathbf{E}[\alpha\,\mathbf{U}\,\alpha]) \,|\, (\mathbf{E}[\alpha\,\mathbf{R}\,\alpha])$$

We extend the basic **CTL** formulas as follows. First, other Boolean operators are viewed as shorthands. For example, $\bot \doteq \neg\top$, $\alpha \vee \beta \doteq \neg(\neg\alpha \wedge \neg\beta)$. Second, we consider

a number of dual temporal operators, whose definition can be obtained by negating the operands and simultaneously replacing $\mathbf{A}$ by $\neg\mathbf{E}$, $\mathbf{U}$ by $\mathbf{R}$, and $\mathbf{R}$ by $\mathbf{U}$.

Definition 4. Extended **CTL** *formulas are the basic* **CTL** *formulas together with (1) ordinary Boolean operators, (2) the following duals:* $\mathbf{AX}\,\alpha \doteq \neg\mathbf{EX}\,\neg\alpha$, $\mathbf{A}[\alpha\,\mathbf{U}\,\beta] \doteq \neg\,\mathbf{E}[\neg\alpha\,\mathbf{R}\,\neg\beta]$, *and* $\mathbf{A}[\alpha\,\mathbf{R}\,\beta] \doteq \neg\,\mathbf{E}[\neg\alpha\,\mathbf{U}\,\neg\beta]$, *and (3) the following particularizations:* $\mathbf{EF}\,\alpha \doteq \mathbf{E}[\top\,\mathbf{U}\,\alpha]$, $\mathbf{EG}\,\alpha \doteq \mathbf{E}[\bot\,\mathbf{R}\,\alpha]$, $\mathbf{AF}\,\alpha \doteq \mathbf{A}[\top\,\mathbf{U}\,\alpha]$, *and* $\mathbf{AG}\,\alpha \doteq \mathbf{A}[\bot\,\mathbf{R}\,\alpha]$.

Mnemotechnically, the letters $\mathbf{E}$ and $\mathbf{A}$ denote *Exists* and *for All*, respectively. The letters $\mathbf{X}$, $\mathbf{U}$, and $\mathbf{R}$, in turn, abbreviate "*neXt* state," "*Until*," and "*Release*," respectively.

Definition 5. *(Semantics)*

- $\mathcal{M} \models_s \top$.
- $\mathcal{M} \models_s p$ *iff* $p \in L(s)$.
- $\mathcal{M} \models_s \neg\alpha$ *iff* $\mathcal{M} \not\models_s \alpha$.
- $\mathcal{M} \models_s \alpha \wedge \beta$ *iff* $\mathcal{M} \models_s \alpha$ *and* $\mathcal{M} \models_s \beta$.
- $\mathcal{M} \models_s \mathbf{EX}\,\alpha$ *iff there exists a path* $s_0, s_1, \ldots$, *where* s_0 *equals* s, *such that* $\mathcal{M} \models_{s_1} \alpha$.
- $\mathcal{M} \models_s \mathbf{E}[\alpha\,\mathbf{U}\,\beta]$ *iff there exists a path* $s_0, s_1, \ldots$, *where* s_0 *equals* s, *and a* $j \geq 0$ *such that for all* $i < j$, *we have* $\mathcal{M} \models_{s_i} \alpha$ *and* $\mathcal{M} \models_{s_j} \beta$.
- $\mathcal{M} \models_s \mathbf{E}[\alpha\,\mathbf{R}\,\beta]$ *iff there exists a path* $s_0, s_1, \ldots$, *where* s_0 *equals* s, *such that either there is some* $i \geq 0$ *such that* $\mathcal{M} \models_{s_i} \alpha$ *and for all* $0 \leq j \leq i$ *we have* $\mathcal{M} \models_{s_j} \beta$, *or for all* $k \geq 0$, *we have* $\mathcal{M} \models_{s_k} \beta$.

In the model $\mathcal{M}_0$ above, for example, $\mathcal{M}_0 \models_{s_0} \mathbf{EX}\,p$ and $\mathcal{M}_0 \models_{s_0} \mathbf{EF}\,p$ hold, but $\mathcal{M}_0 \models_{s_0} p$ does not. In addition, $\mathcal{M}_0 \models_{s_1} \mathbf{EG}\,p$ and $\mathcal{M}_0 \models_{s_0} \mathbf{EX}\,\mathbf{AG}\,p$ hold, but $\mathcal{M}_0 \models_{s_0} \mathbf{AG}\,p$ does not.

Negation Normal Form

Given a Kripke structure $\mathcal{M} = \langle S, R, L\rangle$, a **CTL** formula α, and a state s, we are interested in modifying R and L, obtaining $\mathcal{M}' = \langle S, R', L'\rangle$, in such a way that $\mathcal{M}' \models_s \alpha$ holds, if possible. Compared with the *model-checking* problem (determining whether or not $\mathcal{M} \models_s \alpha$ holds) we have an important variation. Sometimes model checkers for **CTL** solve the more general problem of computing *all* states s of the model $\mathcal{M}$ satisfying α (Huth & Ryan 2004, p 222). This allows the possibility of viewing *negation* as the *set difference* w.r.t. the set of states of the model.

In our case, computing the set of all models $\mathcal{M}'$ with the same set S of states, such that $\mathcal{M}' \models_s \alpha$ holds, would also allow us to view negation as set difference, but would be intolerably inefficient, as there is a vast number of such models. Consequently, we will not treat arbitrary occurrences of negation. By contrast, if we limit ourselves to negation applied to atomic formulas, it is possible to treat negation directly, as we will see. This implies, however, having to transform arbitrary **CTL** formulas to "Negation Normal Form."

Definition 6. *An extended* **CTL** *formula is in* Negation Normal Form *(***NNF***) iff "¬" is applied only to atomic formulas.*

NNF can be readily obtained by repetitively pushing the negation symbol to the atomic level and replacing each operator by its dual. For instance $\neg\mathbf{EX}\,p$ is converted to $\mathbf{AX}\,\neg p$. It is easy to see that this process obtains an **NNF** formula equivalent to a given **CTL** formula.

A model-checking or model-synthesis algorithm would have as input a formula in **NNF**. Hence, such an algorithm must treat the dual operators as primitive operators.

The following equivalences (Clarke, Grumberg, & Peled 1999, p 63), (Huth & Ryan 2004, p 217) are instrumental for such a model-checking or model-synthesis algorithm:

$$\mathbf{E}[\alpha\,\mathbf{U}\,\beta] \equiv \beta \vee (\alpha \wedge \mathbf{EX}\;\mathbf{E}[\alpha\,\mathbf{U}\,\beta]) \quad (1)$$

$$\mathbf{E}[\alpha\,\mathbf{R}\,\beta] \equiv \beta \wedge (\alpha \vee \mathbf{EX}\;\mathbf{E}[\alpha\,\mathbf{R}\,\beta]) \quad (2)$$

$$\mathbf{A}[\alpha\,\mathbf{U}\,\beta] \equiv \beta \vee (\alpha \wedge \mathbf{AX}\;\mathbf{A}[\alpha\,\mathbf{U}\,\beta]) \quad (3)$$

$$\mathbf{A}[\alpha\,\mathbf{R}\,\beta] \equiv \beta \wedge (\alpha \vee \mathbf{AX}\;\mathbf{A}[\alpha\,\mathbf{R}\,\beta]) \quad (4)$$

These apparently circular definitions can be used to define the four operators on the left in terms of $\mathbf{EX}$ and $\mathbf{AX}$ by means of *fixed points* of predicate transformers. The resulting algorithm computes all the states of the model in which a formula holds.

Alternatively, we could also compute one state at a time, and use a cycle-detection mechanism, instead of fixed points. Our model-synthesis method will parallel such a model-checking algorithm.

Explanations

In **CTL** model checking, counterexamples are generated only for "universal" **CTL** formulas, i.e. those with operators starting with an $\mathbf{A}$. Consider for example $\mathbf{AF}\,\alpha$, which holds in state s iff for all paths starting in s there is some state in which α holds. If $\mathbf{AF}\,\alpha$ does not hold in state s, then there is a path starting in s such that α is false in all states of such a path. This path will be a counterexample.

Consider by contrast $\mathbf{EF}\,\alpha$, which holds in state s iff there is a path starting in s having a state in which α holds. If $\mathbf{EF}\,\alpha$ does not hold in state s, then there is no path starting in s having a state in which α is true. Therefore, all paths starting in s will be counterexamples. Instead of generating any one such path, the NuSMV model checker, for instance, gives more information by returning s only. In case of formulas with nested universal and existential operators, NuSMV produces a path prefix ending in a state in which the outermost existential formula does not hold. As a result, universal operators occurring inside an existential operator provide no information to the counterexample. This drawback of counterexamples suggests considering "explanations" instead.

Following the **CTL** model-checking algorithms of (Huth & Ryan 2004), we can learn first the smallest subformulas and work towards the main formula. Explanations allow us to learn *conjunctions* $\alpha \wedge \beta$ of formulas as follows. We first inductively learn α. Next, we find an explanation for α and "protect" such an explanation. Finally, we learn β in such a way that the explanation for α is preserved. (Learning β might involve the addition or removal of transitions or labels.) We will then have learned both conjuncts.

An algorithm for computing explanations

Let us consider a possible definition of explanations. Given a model $\mathcal{M} = \langle S, R, L\rangle$ in which a formula α holds, an explanation for α would be a minimal part of the model that makes α true.

Take for instance the model $\mathcal{M}_0$ above. An explanation for the truth of p at the state s_1 of $\mathcal{M}_0$ given that $\mathcal{M}_0 \models_{s_1} p$ holds, would be the label p in state s_1. Hence, for representing explanations for atomic formulas (i.e. positive literals), we need $L' \subseteq S \times \mathrm{Prop}$.

In the case of a negative literal, consider $\mathcal{M}_0 \models_{s_0} \neg p$. If we record the occurrence of *negative* literals in states (i.e. $(s_0, \neg p)$), we will have a symmetrical situation to that of positive literals, and we will be able to handle negation (of atomic formulas). Hence, in addition to recording positive, we will record negative literals: $L' \subseteq S \times \mathrm{Lit}$, where Lit is the set of literals of Prop.

In the case of a conjunction $\alpha \wedge \beta$, we would need to explain first α, then β, and finally obtain the "union" of both explanations. As we have not yet finished describing the components of an explanation, we will relegate the definition of explanation union to the end of this section.

Let us consider now a disjunction $\alpha \vee \beta$. If only one of α or β holds, we inductively explain the subformula that holds. If both hold, however, we have a nondeterministic choice, as we will be able to explain $\alpha \vee \beta$ by explaining either α or β, but it is not possible to know a priori which of the two explanations will be needed for learning. Our definition of an explanation will therefore be a "nondeterministic" function.

Consider now $\mathbf{EX}\,\alpha$. An explanation for $\mathcal{M}_0 \models_{s_0} \mathbf{EX}\,p$, say, would be the transition from s_0 to s_1 together with the explanation for p in s_1. Hence, in addition to L' we need a second component of explanations recording transitions, i.e. $R' \subseteq R$. Moreover, since in general a state can have several successors in which α holds, we nondeterministically choose any such successor.

Next, we deal with $\mathbf{AX}\,\alpha$. At first sight it might appear that we need *all* successors of the state s in which α holds to explain why such a formula holds. However, a closer look will reveal that we need only *one* successor. The reason is that we can remove (as a result of the learning subsequent subformulas) all transitions coming out of s except for one, and $\mathbf{AX}\,\alpha$ will still hold. An explanation for this operator will then be similar to that of $\mathbf{EX}\,\alpha$. A difference is that we must also recall that subsequent learning can add transitions coming out of s, provided that such transitions go to states in which α holds. Hence, we need a third component for explanations, consisting of a set of (s, α)-pairs: $S' \subseteq S \times \mathbf{NNF}$.

As with the model-checking problem for **NNF** formulas, explanations for the rest of the operators, $\mathbf{EU}$, $\mathbf{ER}$, $\mathbf{AU}$, and $\mathbf{AR}$ can be obtained using the equivalences (1–4), together with a cycle-detection mechanism.

As a consequence, an *explanation* is a tuple $\langle S', R', L'\rangle$, where $S' \subseteq S \times \mathbf{NNF}$, $R' \subseteq R$, and $L' \subseteq S \times \mathrm{Lit}$. Throughout, E will denote explanations.

The union of two explanations, $\uplus : \mathrm{Expl}^2 \to \mathrm{Expl}$, is $\langle S_1, R_1, L_1\rangle \uplus \langle S_2, R_2, L_2\rangle = \langle S_1 \cup S_2, R_1 \cup R_2, L_1 \cup L_2\rangle$.

Finally, we deal with $\top$ and $\bot$. The explanation for $\top$, the identity for conjunction, is the identity for the union of explanations, i.e. the *empty explanation* $\langle \emptyset, \emptyset, \emptyset\rangle$. The explanation for $\bot$, the identity for disjunction, is the identity for nondeterministic choice, i.e. the *undefined explanation* $E_\bot$.

Model synthesis

Having outlined an algorithm for computing explanations, we now turn our attention to learning subformulas given an explanation of subformulas already learned.

An algorithm for synthesizing models

Learning α given $\mathcal{M}$, E, and s, will mean finding a model $\mathcal{M}'$ "similar" to $\mathcal{M}$, such that $\mathcal{M}' \models_s \alpha$, provided that $\mathcal{M}'$ is "compatible" with E, if possible.

First, we must determine whether or not $\mathcal{M} \models_s \alpha$. If the answer is positive, $\mathcal{M}'$ is $\mathcal{M}$. (Note that this covers $\alpha = \top$.) If the answer is negative, we treat the following cases.

A positive literal p can be learned only by adding p to s, provided that E does not have $\neg p$ in s. Symmetrically, a negative literal $\neg p$ can be learned only by adding $\neg p$ to s, provided that E does not have p in s.

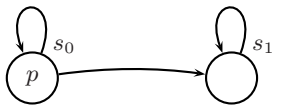
We now consider a conjunction $\alpha \wedge \beta$. First, we inductively learn α given $\mathcal{M}$, E, and s, obtaining a model $\mathcal{M}''$. Next, we nondeterministically find an explanation E' for α. Finally, we inductively learn β given $\mathcal{M}''$, $E \uplus E'$, and s, if possible.

A disjunction $\alpha \vee \beta$, in turn, can be learned by nondeterministically learning one of α or β.

Now we deal with $\mathbf{EX}\,\alpha$ and $\mathbf{AX}\,\alpha$, for which we will use the following model $\mathcal{M}_1$:

Assume that we wish to learn $\mathbf{EX}\,p$ at s_0. One possibility is to learn p at s_1:

It may be the case that the given explanation of previously learned conjuncts might prevent us from learning p at s_1. Therefore, we must also consider another way of making $\mathbf{EX}\,p$ hold at s_0, namely, making s_0 a successor of itself:



In general, the given explanation might prevent us from learning α in any state. Consequently, we must allow for nondeterministically learning α in any state. If such a state is not a successor, we must also add a transition, if possible. In this last case, it is important to first add the transition and then learn α at the non-successor.

Consider next $\mathbf{AX}\,\alpha$. Suppose that we are to learn $\mathbf{AX}\,p$ at s_0 in $\mathcal{M}_1$. A first way would again be to learn p at s_1:

If it is not possible to do so, we could also *eliminate* s_1 as a successor of s_0 by deleting the transition from s_0 to s_1. This example illustrates that such a deletion may result in a non-total relation, as s_0 has no successors. To make the new relation total, we can learn p at a state that was not a successor of s_0 before the deletion (s_0 in this model), and add a transition.

In general, for each successor s' of s, we nondeterministically either learn α at such a successor, or eliminate s' as successor of s. In case s ends up with no successors after the eliminations, we learn α at any state which was not a successor and add a transition.

In a manner similar to that of model checking and explanations for **NNF** formulas, we can employ the equivalences (1–4), together with a cycle-detection mechanism.

The URL `leibniz.iimas.unam.mx/~drosenbl/ctl_learning` has a formalization of this learning-algorithm sketch together with a Prolog implementation.

Related work

This section summarizes a model-synthesis method (Calzone *et al.* 2006) for **CTL**. This method is part of the Biocham system for modeling biochemical networks.

Unlike our method, Biocham's learning algorithm is based on counterexamples. Assume that $\mathcal{M} \models_s \alpha$ does not hold, and that we wish to modify $\mathcal{M}$ so that it does. If α contains only non-negated *universal* temporal operators, a counterexample computed by a model checker represents a path that makes α false. Biocham, therefore, deletes transitions occurring in such a path. If the deletion produces an accessibility relation which is not total, leaving a state with no successors, then a loop at that state is added.

If α contains only non-negated *existential* temporal operators, a counterexample will not be produced, as we observed at the beginning of the section "Explanations." Biocham, however, can add transitions using a bias taken from the application domain.

Formulas that have both universal and existential operators, i.e. "unclassified" formulas, are treated by adding and deleting transitions using a counterexample. Such a counterexample, as we saw, only provides information about the outermost universal operators of the formula. Again Biocham can add transitions using a bias.

Existential formulas are treated first, then the unclassified ones, and finally the universal ones. The deletions for satisfying universal formulas are allowed to dissatisfy some existential or unclassified formulas, in which case such formulas are treated again, this time not dissatisfying the universal formulas already satisfied. Presumably existential formulas are treated first because, as universal formulas are treated with deletions, we would otherwise produce a "poor" model.

Compared with our method, Biocham has the advantage of being based on NuSMV, a well-established model checker. A drawback of Biocham, however, is that counterexamples only provide information about the outermost universal operators of the formula. All other occurrences of operators are treated with heuristics.

Concluding remarks

Model checking is arguably the most successful formal technique for designing complex digital systems. A reason is that unlike other formal techniques performing complete verifications, model checking concentrates on debugging. At the same time, model checking is often superior to more conventional methods such as testing dealing with individual input-output pairs: model checking proves the presence or absence of *properties*, such as security, fairness or deadlock freedom, expressed as formulas in a temporal logic.

When a model lacks a desired property, model checkers typically give a *counterexample* showing why the property does not hold. This counterexample serves as a guide for manually modifying the faulty model. Counterexamples, however, are limited in that they are restricted to universal formulas, for example.

We provided an automatic method based on *explanations* instead, applicable to formulas in computation-tree logic. An important question is whether or not our method is complete in the sense that if a model satisfying the desired property exists, then our method finds such a model. We are currently working on this problem.

Acknowledgments

We gratefully acknowledge stimulating discussions with Elena Alvarez-Buylla's group, the facilities at IIMAS, UNAM, and Carlos Velarde's help with the figures.

References

Bryant, R. E. 1992. Symbolic Boolean manipulation with ordered binary-decision diagrams. *ACM Computing Surveys* 24(3):293–318.

Calzone, L.; Chabrier-Rivier, N.; Fages, F.; and Soliman, S. 2006. Machine learning biochemical networks from temporal logic properties. In *Transactions on Computational Systems Biology VI*, 68–94. LNBI No. 4220.

Chabrier-Rivier, N.; Chiaverini, M.; Danos, V.; Fages, F.; and Schächter, V. 2004. Modeling and querying biomolecular interaction networks. *TCS* 325:25–44.

Clarke, E. M.; Grumberg, O.; and Peled, D. A. 1999. *Model Checking*. MIT Press.

Espinosa-Soto, C.; Padilla-Longoria, P.; and Alvarez-Buylla, E. 2004. A gene regulatory network model for cell-fate determination during *Arabidopsis thaliana* flower development that is robust and recovers experimental gene expression profiles. *The Plant Cell* 16:2923–2939.

Huth, M. R. A., and Ryan, M. D. 2004. *Logic in Computer Science*. Cambridge University Press, 2nd edition.