Grey-Box Learning of Register Automata

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Abstract. Model learning (a.k.a. active automata learning) is a highly effective technique for obtaining black-box finite state models of software components. Thus far, generalization to infinite state systems with inputs and outputs that carry data parameters has been challenging. Existing model learning tools for infinite state systems face scalability problems and can only be applied to restricted classes of systems (register automata with equality/inequality). In this article, we show how one can boost the performance of model learning techniques by extracting the constraints on input and output parameters from a run, and making this grey-box information available to the learner. More specifically, we provide new implementations of the tree oracle and equivalence oracle from the RALib tool, which use the derived constraints. We extract the constraints from runs of Python programs using an existing tainting library for Python, and compare our grey-box version of RALib with the existing black-box version on several benchmarks, including some data structures from Python’s standard library. Our proof-of-principle implementation results in almost two orders of magnitude improvement in terms of numbers of inputs sent to the software system. Our approach, which can be generalized to richer model classes, also enables RALib to learn models that are out of reach of black-box techniques, such as combination locks.

Keywords: Model learning · Active Automata Learning · Register Automata · RALib · Grey-box · Tainting

1 Introduction

Model learning, also known as active automata learning, is a black-box technique for constructing state machine models of software and hardware components from information obtained through testing (i.e., providing inputs and observing the resulting outputs). Model learning has been successfully used in numerous applications, for instance for generating conformance test suites of software components [13], finding mistakes in implementations of security-critical protocols [8–10], learning interfaces of classes in software libraries [14], and checking that

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a legacy component and a refactored implementation have the same behaviour [19]. We refer to [17, 20] for surveys and further references.

In many applications it is crucial for models to describe control flow, i.e., states of a component, data flow, i.e., constraints on data parameters that are passed when the component interacts with its environment, as well as the mutual influence between control flow and data flow. Such models often take the form of extended finite state machines (EFSMs). Recently, various techniques have been employed to extend automata learning to a specific class of EFSMs called register automata, which combine control flow with guards and assignments to data variables [1, 2, 6].

While these works demonstrate that it is theoretically possible to infer such richer models, the presented approaches do not scale well and are not yet satisfactorily developed for richer classes of models (c.f. [16]): Existing techniques either rely on manually constructed mappers that abstract the data aspects of input and output symbols into a finite alphabet, or otherwise infer guards and assignments from black-box observations of test outputs. The latter can be costly, especially for models where control flow depends on test on data parameters in input: in this case, learning an exact guard that separates two control flow branches may require a large number of queries.

One promising strategy for addressing the challenge of identifying data-flow constraints is to augment learning algorithms with white-box information extraction methods, which are able to obtain information about the System Under Test (SUT) at lower cost than black-box techniques. Several researchers have explored this idea. Giannakopoulou et al. [11] develop an active learning algorithm that infers safe interfaces of software components with guarded actions. In their model, the teacher is implemented using concolic execution for the identification of guards. Cho et al. [7] present MACE an approach for concolic exploration of protocol behaviour. The approach uses active automata learning for discovering so-called deep states in the protocol behaviour. From these states, concolic execution is employed in order to discover vulnerabilities. Similarly, Botičan and Babić [4] present a learning algorithm for inferring models of stream transducers that integrates active automata learning with symbolic execution and counterexample-guided abstraction refinement. They show how the models can be used to verify properties of input sanitizers in Web applications. Finally, Howar et al. [15] extend the work of [11] and integrate knowledge obtained through static code analysis about the potential effects of component method invocations on a component’s state to improve the performance during symbolic queries. So far, however, white-box techniques have never been integrated with learning algorithms for register automata.

In this article, we present the first active learning algorithm for a general class of register automata that uses white-box techniques. More specifically, we show how dynamic taint analysis can be used to efficiently extract constraints on input and output parameters from a test, and how these constraints can be used to improve the performance of the \( SL^* \) algorithm of Cassel et al. [6]. The \( SL^* \) algorithm generalizes the classical \( L^* \) algorithm of Angluin [3] and has
been used successfully to learn register automaton models, for instance of Linux and Windows implementations of TCP [9]. We have implemented the presented method on top of RALib [5], a library that provides an implementation of the $SL^*$ algorithm.

The integration of the two techniques (dynamic taint analysis and learning of register automata models) can be explained most easily with reference to the architecture of RALib, shown in Figure 1, which is a variation of the Minimally Adequate Teacher (MAT) framework of [3]: In the MAT framework, learning is viewed as a game in which a learner has to infer the behaviour of an unknown register automaton $M$ by asking queries to a teacher. We postulate $M$ models the behaviour of a System Under Test (SUT). In the learning phase, the learner (that is, $SL^*$) is allowed to ask questions to the teacher in the form of tree queries (TQs) and the teacher responds with symbolic decision trees (SDTs). In order to construct these SDTs, the teacher uses a tree oracle, which queries the SUT with membership queries (MQs) and receives a yes/no reply to each. Typically, the tree oracle asks multiple MQs to answer a single tree query in order to infer causal impact and flow of data values. Based on the answers on a number of tree queries, the learner constructs a hypothesis in the form of a register automaton $H$. The learner submits $H$ as an equivalence query (EQ) to the teacher, asking whether $H$ is equivalent to the SUT model $M$. The teacher uses an equivalence oracle to answer equivalence queries. Typically, the equivalence oracle asks multiple MQs to answer a single equivalence query. If, for all membership queries, the output produced by the SUT is consistent with hypothesis $H$, the answer to the equivalence query is ‘Yes’ (indicating learning is complete). Otherwise, the answer ‘No’ is provided, together with a counterexample (CE) that indicates a difference between $H$ and $M$. Based on this CE, learning continues. In this extended MAT
framework, we have constructed new implementations of the tree oracle and equivalence oracle that leverage the constraints on input and output parameters that are imposed by a program run: dynamic tainting is used to extract the constraints on parameters that are encountered during a run of a program. Our implementation learns models of Python programs, using an existing tainting library for Python [12]. Effectively, the combination of the $SL^*$ with our new tree and equivalence oracles constitutes a grey-box learning algorithm, since we only give the learner partial information about the internal structure of the SUT.

We compare our grey-box tree and equivalence oracles with the existing black-box versions of these oracles on several benchmarks, including Python’s queue and set modules. Our proof-of-concept implementation results in almost two orders of magnitude improvement in terms of numbers of inputs sent to the software system. Our approach, which generalises to richer model classes, also enables RALib to learn models that are completely out of reach for black-box techniques, such as combination locks.

**Outline:** Section 2 contains preliminaries; Section 3 discusses tainting in our Python SUTs; Section 4 contains the algorithms we use to answer TQs using tainting and the definition for the tainted equivalence oracle needed to learn combination lock automata; Section 5 contains the experimental evaluation of our technique; and Section 6 concludes.

## 2 Preliminary definitions and constructions

This section contains the definitions and constructions necessary to understand active automata learning for models with dataflow. We first define the concept of a *structure*, followed by *guards*, *data languages*, *register automata*, and finally *symbolic decision trees*.

**Definition 1 (Structure).** A structure $S = \langle R, D, r \rangle$ is a triple where $R$ is a set of relation symbols, each equipped with an arity, $D$ is an infinite domain of data values, and $r$ contains a distinguished $n$-ary relation symbol $r^R \subseteq D^n$ for each $n$-ary relation symbol $r \in R$.

In the remainder of this article, we fix a structure $S = \langle R, D, r \rangle$, where $R$ contains a binary relation symbol $=$ and unary relation symbols $= c$, for each $c$ contained in a finite set $C$ of constant symbols, $D$ equals the set $\mathbb{N}$ of natural numbers, $=^R$ is interpreted as the equality predicate on $\mathbb{N}$, and to each symbol $c \in C$ a natural number $n_c$ is associated such that $(= c)^R = \{n_c\}$.

Guards are a restricted type of Boolean formulas that may contain relation symbols from $R$.

**Definition 2 (Guards).** We postulate a countably infinite set $V = \{v_1, v_2, \ldots\}$ of variables. In addition, there is a variable $p \notin V$ that will play a special role as formal parameter of input symbols; we write $V^+ = V \cup \{p\}$. A guard is

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3 Available at [https://bitbucket.org/toonlenaerts/taintralib/src/basic.](https://bitbucket.org/toonlenaerts/taintralib/src/basic.)
We require that \( M \) (denoted by a double circle), and one rejecting “sink” location \( X \) contained in \( X \) is a tautology. Let \( \alpha \) and input symbol \( \Sigma \) actions i.e., \( \alpha \) -transitions out of a location, the disjunction of the guards of the \( \alpha \) -transitions with source \( l \) are called guards. Function \( g \) maps each location in \( L \) to either accepting (\( + \)) or rejecting (\( - \)).

Next, we define the notion of a data language. For this, we fix a finite set of actions \( \Sigma \). A data symbol \( \alpha(d) \) is a pair consisting of an action \( \alpha \in \Sigma \) and a data value \( d \in D \). While relations may have arbitrary arity, we will assume that all actions have an arity of one to ease notation and simplify the text. A data word is a finite sequence of data symbols, and a data language is a set of data words. We denote concatenation of data words \( w \) and \( w' \) by \( w \cdot w' \), where \( w \) is the prefix and \( w' \) is the suffix. \( \text{Acts}(w) \) denotes the sequence of actions \( \alpha_1 \alpha_2 \ldots \alpha_n \) in \( w \), and \( \text{Vals}(w) \) denotes the sequence of data values \( d_1 d_2 \ldots d_n \) in \( w \). We refer to a sequence of actions in \( \Sigma^* \) as a symbolic suffix. If \( w \) is a symbolic suffix then we write \( \| w \| \) for the set of data words \( u \) with \( \text{Acts}(u) = w \).

Data languages may be represented by register automaton, defined below.

**Definition 3 (Register Automaton)**. A Register Automaton (RA) is a tuple \( \mathcal{M} = (L, l_0, \mathcal{X}, \Gamma, \lambda) \) where

- \( L \) is a finite set of locations, with \( l_0 \) as the initial location;
- \( \mathcal{X} \) maps each location \( l \in L \) to a finite set of registers \( \mathcal{X}(l) \);
- \( \Gamma \) is a finite set of transitions, each of the form \( \langle l, \alpha(p), g, \pi, l' \rangle \), where
  - \( l, l' \) are source and target locations respectively,
  - \( \alpha(p) \) is a parametrised action,
  - \( g \) is a guard over \( \mathcal{X}(l) \cup \{ p \} \), and
  - \( \pi \) is an assignment mapping from \( \mathcal{X}(l') \) to \( \mathcal{X}(l) \cup \{ p \} \); and
- \( \lambda \) maps each location in \( L \) to either accepting (\( + \)) or rejecting (\( - \)).

We require that \( \mathcal{M} \) is deterministic in the sense that for each location \( l \in L \) and input symbol \( \alpha \in \Sigma \), the conjunction of the guards of any pair of distinct \( \alpha \)-transitions with source \( l \) is not satisfiable. \( \mathcal{M} \) is completely specified if for all \( \alpha \)-transitions out of a location, the disjunction of the guards of the \( \alpha \)-transitions is a tautology. \( \mathcal{M} \) is said to be simple if there are no registers in the initial location, i.e., \( \mathcal{X}(l_0) = \emptyset \). In this text, all RAs are assumed to be completely specified and simple, unless explicitly stated otherwise. Locations \( l \in L \) with \( \lambda(l) = + \) are called accepting, and locations with \( \lambda(l) = - \) are rejecting.

**Example 1 (FIFO-buffer)**. The register automaton displayed in Figure 2 models a FIFO-buffer with capacity 2. It has three accepting locations \( l_0, l_1 \) and \( l_2 \) (denoted by a double circle), and one rejecting “sink” location \( l_3 \) (denoted by a single circle). Function \( \mathcal{X} \) assigns the empty set of registers to locations \( l_0 \) and \( l_3 \), singleton set \( \{ x \} \) to location \( l_1 \), and set \( \{ x, y \} \) to \( l_2 \).
2.1 Semantics of a RA

We now formalise the semantics of an RA. A valuation of a set of variables $X$ is a function $\nu : X \rightarrow D$ that assigns data values to variables in $X$. If $\nu$ is a valuation of $X$ and $g$ is a guard over $X$ then $\nu \models g$ is defined inductively by:

- $\nu \models r(x_1, \ldots, x_n)$ iff $(\nu(x_1), \ldots, \nu(x_n)) \in r^R$
- $\nu \models \neg r(x_1, \ldots, x_n)$ iff $(\nu(x_1), \ldots, \nu(x_n)) \notin r^R$
- $\nu \models g_1 \land g_2$ iff $\nu \models g_1$ and $\nu \models g_2$

A state of a RA $M = (L, l_0, X, \Gamma, \lambda)$ is a pair $\langle l, \nu \rangle$, where $l \in L$ is a location and $\nu : X(l) \rightarrow D$ is a valuation of the set of registers at location $l$. A run of $M$ over data word $w = \alpha_1(d_1) \ldots \alpha_n(d_n)$ is a sequence

$$\langle l_0, \nu_0 \rangle \xrightarrow{\alpha_1(d_1), g_1, \pi_1} \langle l_1, \nu_1 \rangle \ldots \langle l_{n-1}, \nu_{n-1} \rangle \xrightarrow{\alpha_n(d_n), g_n, \pi_n} \langle l_n, \nu_n \rangle,$$

where

- for each $0 \leq i \leq n$, $\langle l_i, \nu_i \rangle$ is a state (with $l_0$ the initial location),
- for each $0 < i \leq n$, $\langle l_{i-1}, \alpha_i(p), g_i, \pi_i, l_i \rangle \in \Gamma$ such that $\xi_i \models g_i$ and $\nu_i = \nu_{i-1} \circ \pi_i$, where $\nu_i = \nu_{i-1} \cup \{[p \mapsto d_i]\}$ extends $\nu_{i-1}$ by mapping $p$ to $d_i$.

A run is accepting if $\lambda(l_n) = +$, else rejecting. The language of $M$, notation $L(M)$, is the set of words $w$ such that $M$ has an accepting run over $w$. Word $w$ is accepted (rejected) under valuation $\nu_0$ if $M$ has an accepting (rejecting) run that starts in state $\langle l_0, \nu_0 \rangle$. 

![Fig. 2: FIFO-buffer with a capacity of 2 modeled as a register automaton.](image)
Example 2. Consider the FIFO-buffer example from Figure 2. This RA has a run

\[
\langle l_0, \nu_0 = [] \rangle \xrightarrow{\text{Push(7), } g_1 \equiv \top, \pi_1 = [x \mapsto p]} \langle l_1, \nu_1 = [x \mapsto 7] \rangle \xrightarrow{\text{Push(7), } g_2 \equiv \top, \pi_2 = [x \mapsto x, y \mapsto p]} \langle l_2, \nu_2 = [x \mapsto 7, y \mapsto 7] \rangle \xrightarrow{\text{Pop(7), } g_3 \equiv \top, \pi_3 = [x \mapsto y]} \langle l_1, \nu_3 = [x \mapsto 7] \rangle \xrightarrow{\text{Push(5), } g_4 \equiv \top, \pi_4 = [x \mapsto x, y \mapsto p]} \langle l_2, \nu_4 = [x \mapsto 7, y \mapsto 5] \rangle \xrightarrow{\text{Pop(7), } g_5 \equiv \top, \pi_5 = [x \mapsto y]} \langle l_1, \nu_5 = [x \mapsto 5] \rangle \xrightarrow{\text{Pop(5), } g_6 \equiv \top, \pi_6 = []} \langle l_0, \nu_6 = [] \rangle
\]

and thus the trace is Push(7) Push(7) Pop(7) Push(5) Pop(7) Pop(7) Pop(5).

\[\]
transitions in the SDT contain an update \( x_3 := p \), and the final transitions an update \( x_4 := p \). For readability, these updates are not displayed in the diagram. The SDT accepts suffixes of form \( \text{Pop}(d_1) \text{Pop}(d_2) \) iff \( d_1 \) equals the value stored in register \( x_1 \), and \( d_2 \) equals the data value stored in register \( x_2 \).

The formal definitions of an SDT and the notion of a tree oracle are presented in Appendix A. For a more detailed discussion of SDTs we refer to [6].

3 Tainting

We postulate that the behaviour of the SUT (in our case: a Python program) can be modeled by a register automaton \( M \). In a black-box setting, observations on the SUT will then correspond to words from the data language of \( M \). In this section, we will describe the additional observations that a learner can make in a grey-box setting, where the constraints on the data parameters that are imposed within a run become visible. In this setting, observations of the learner will correspond to what we call tainted words of \( M \). Tainting semantics is an extension of the standard semantics in which each input value is “tainted” with a unique marker from \( V \). In a data word \( w = \alpha_1(d_1)\alpha_2(d_2)\ldots\alpha_n(d_n) \), the first data value \( d_1 \) is tainted with marker \( v_1 \), the second data value \( d_2 \) with \( v_2 \), etc. While the same data value may occur repeatedly in a data word, all the markers are different.

3.1 Semantics of Tainting

A tainted state of a RA \( M = (L, l_0, X, \Gamma, \lambda) \) is a triple \( \langle l, \nu, \zeta \rangle \), where \( l \in L \) is a location, \( \nu : X(l) \rightarrow D \) is a valuation, and \( \zeta : X(l) \rightarrow V \) is a function that assigns a marker to each register of \( l \). A tainted run of \( M \) over data word \( w = \alpha_1(d_1)\ldots\alpha_n(d_n) \) is a sequence

\[ \tau = \langle l_0, \nu_0, \zeta_0 \rangle \xrightarrow{\alpha_1(d_1), g_1, \pi_1} \langle l_1, \nu_1, \zeta_1 \rangle \ldots \xrightarrow{\alpha_n(d_n), g_n, \pi_n} \langle l_n, \nu_n, \zeta_n \rangle, \]

where

- \( \langle l_0, \nu_0 \rangle \xrightarrow{\alpha_1(d_1), g_1, \pi_1} \langle l_1, \nu_1, \zeta_1 \rangle \ldots \xrightarrow{\alpha_n(d_n), g_n, \pi_n} \langle l_n, \nu_n, \zeta_n \rangle \) is a run of \( M \),
- for each \( 0 \leq i \leq n \), \( \langle l_i, \nu_i, \zeta_i \rangle \) is a tainted state,
- for each \( 0 < i \leq n \), \( \zeta_i = \kappa_i \circ \pi_i \), where \( \kappa_i = \zeta_{i-1} \cup \{ (p, v_i) \} \).

The tainted word of \( \tau \) is the sequence \( w = \alpha_1(d_1)G_1\alpha_2(d_2)G_2\ldots\alpha_n(d_n)G_n \), where \( G_i = g_i[\kappa_i] \), for \( 0 < i \leq n \). We define \( \text{constraints}_M(\tau) = [G_1, \ldots, G_n] \).

Let \( w = \alpha_1(d_1)\ldots\alpha_n(d_n) \) be a data word. Since register automata are deterministic, there is a unique tainted run \( \tau \) over \( w \). We define \( \text{constraints}_M(w) = \text{constraints}_M(\tau) \), that is, the constraints associated to a data word are the constraints of the unique tainted run that corresponds to it. In the untainted setting a membership query for data word \( w \) leads to a response “yes” if \( w \in L(M) \), and a response “no” otherwise, but in a tainted setting the predicates \( \text{constraints}_M(w) \) are also included in the response, and provide additional information that the learner may use.
Example 3. Consider the FIFO-buffer example from Figure 2. This RA has a tainted run

$\langle l_0, [], [] \rangle \xrightarrow{\text{Push}(7)} \langle l_1, [x \mapsto 7], [x \mapsto v_1] \rangle \xrightarrow{\text{Push}(7)} \langle l_2, [x \mapsto 7, y \mapsto 7], [x \mapsto v_1, y \mapsto v_2] \rangle \xrightarrow{\text{Pop}(7)} \langle l_1, [x \mapsto 7], [x \mapsto v_2] \rangle \xrightarrow{\text{Push}(5)} \langle l_2, [x \mapsto 7, y \mapsto 5], [x \mapsto v_2, y \mapsto v_4] \rangle \xrightarrow{\text{Pop}(7)} \langle l_1, [x \mapsto 5], [y \mapsto v_4] \rangle \xrightarrow{\text{Pop}(5)} \langle l_0, [], [] \rangle$

(For readability, guards $g_i$ and assignments $\pi_i$ have been left out.) The constraints in the corresponding tainted trace can be computed as follows:

- $\kappa_1 = [p \mapsto v_1]$ \hspace{1cm} $G_1 \equiv T[\kappa_1] \equiv T$
- $\kappa_2 = [x \mapsto v_1, p \mapsto v_2]$ \hspace{1cm} $G_2 \equiv T[\kappa_2] \equiv T$
- $\kappa_3 = [x \mapsto v_1, y \mapsto v_2, p \mapsto v_3]$ \hspace{1cm} $G_3 \equiv (p = x)[\kappa_3] \equiv v_3 = v_1$
- $\kappa_4 = [x \mapsto v_2, p \mapsto v_4]$ \hspace{1cm} $G_4 \equiv T[\kappa_4] \equiv T$
- $\kappa_5 = [x \mapsto v_2, y \mapsto v_4, p \mapsto v_5]$ \hspace{1cm} $G_5 \equiv (p = x)[\kappa_5] \equiv v_5 = v_2$
- $\kappa_6 = [x \mapsto v_4, p \mapsto v_6]$ \hspace{1cm} $G_6 \equiv (p = x)[\kappa_6] \equiv v_6 = v_4$

and thus the tainted word is:

$\text{Push}(7) \top \text{Push}(7) \top \text{Pop}(7) \ v_3 = v_1 \top \text{Push}(5) \ v_5 = v_2 \top \text{Pop}(5) \ v_6 = v_4.$

and the corresponding list of constraints is $[\top, \top, v_3 = v_1, \top, v_5 = v_2, \top, v_6 = v_4]$. 

Various techniques can be used to observe tainted traces, for instance symbolic and concolic execution. In this work, we have used a library called “\texttt{taintedstr}” to achieve tainting in Python and make tainted traces available to the learner.

3.2 Tainting in Python

Tainting in Python is achieved by using a library called “\texttt{taintedstr}”\textsuperscript{4}, which implements a “\texttt{tstr}” (tainted string) class. We do not discuss the entire implementation in detail, but only introduce the portions relevant to our work. The “\texttt{tstr}” class works by operator overloading: each operator is overloaded to record its own invocation. The \texttt{tstr} class overloads the implementation of the “\_\_eq\_\_” (equality) method in Python’s \texttt{str} class, amongst others. In this text, we only consider the equality method. A \texttt{tstr} object $x$ can be considered as a triple $\langle o, t, cs \rangle$, where $o$ is the (base) string object, $t$ is the taint value associated with string $o$, and $cs$ is a set of comparisons made by $x$ with other objects, where each comparison $c \in cs$ is a triple $\langle f, a, b \rangle$ with $f$ the name of the binary method invoked on $x$, $a$ a copy of $x$, and $b$ the argument supplied to $f$.

Each a method $f$ in the \texttt{tstr} class is an overloaded implementation of the relevant (base) method $f$ as follows:

\footnote{See [12] and https://github.com/vrthra/taintedstr.}
```python
def f(self, other):
    self.cs.add((m._name_, self, other))
    return self.o.f(other)  # 'o' is the base string
```

We present a short example of how such an overloaded method would work below:

**Example 4 (tstr tainting).** Consider two tstr objects: \( x_1 = \langle '1', 1, \emptyset \rangle \) and \( x_2 = \langle '1', 2, \emptyset \rangle \). Calling \( x_1 == x_2 \) returns \textbf{True} as \( x_1.o = x_2.o \). As a side-effect of \( f \), the set of comparisons \( x_1.cs \) is updated with the triple \( c = \langle \text{"eq"}, x_1, x_2 \rangle \).

We may then confirm that \( x_1 \) is compared to \( x_2 \) by checking the taint values of the variables in comparison \( c: x_1.t = 1 \) and \( x_2.t = 2 \).

Note, our approach to tainting limits the recorded information to operations performed on a tstr object.

**Example 5 (Complicated Comparison).** Consider the following snippet, where \( x_1, x_2, x_3 \) are tstr objects with 1, 2, 3 as taint values respectively:

```python
if not (x_1 == x_2 or (x_2 != x_3)):
    # do something
```

If the base values of \( x_1 \) and \( x_2 \) are equal, the Python interpreter will “short-circuit” the if-statement and the second condition, \( x_2 \neq x_3 \), will not be evaluated. Thus, we only obtain one comparison: \( x_1 = x_2 \). On the other hand, if the base values of \( x_1 \) and \( x_2 \) are not equal, the interpreter will not short-circuit, and both comparisons will be recorded as \{ \( x_2 = x_3, x_1 \neq x_2 \) \}. While the comparisons are stored as a set, from the perspective of the tainted trace, the guard(s) is a single conjunction: \( x_2 = x_3 \land x_1 \neq x_2 \). However, the external negation operation will not be recorded by any of the tstr objects: the negation was not performed on the tstr objects.

4 Learning Register Automata using Tainting

Given an SUT and a tree query, we generate an SDT in the following steps: (i) construct a characteristic predicate of the tree query (Algorithm 1) using membership and guard queries, (ii) transform the characteristic predicate into an SDT (Algorithm 2), and (iii) minimise the obtained SDT (Algorithm 3).

4.1 Tainted Tree Oracle

**Construction of Characteristic Predicate** For \( u = \alpha(d_1) \cdots \alpha_k(d_k) \) a data word, \( \nu_u \) denotes the valuation of \( \{x_1, \ldots, x_k\} \) with \( \nu_u(x_i) = d_i \), for \( 1 \leq i \leq k \). Suppose \( u \) is a prefix and \( w = \alpha_{k+1} \cdots \alpha_{k+n} \) is a symbolic suffix. Then \( H \) is a characteristic predicate for \( u \) and \( w \) in \( \mathcal{M} \) if, for each valuation \( \nu \) of \( \{x_1, \ldots, x_{k+n}\} \) that extends \( \nu_u \),

\[
\nu \models H \iff \alpha_1(\nu(x_1)) \cdots \alpha_{k+n}(\nu(x_{k+n})) \in L(\mathcal{M}),
\]

\[\quad \text{for each valuation } \nu \text{ of } \{x_1, \ldots, x_{k+n}\} \text{ that extends } \nu_u,\]

\[\nu \models H \iff \alpha_1(\nu(x_1)) \cdots \alpha_{k+n}(\nu(x_{k+n})) \in L(\mathcal{M}),\]
Algorithm 1: ComputeCharacteristicPredicate

Data: A tree query consisting of prefix $u = \alpha_1(d_1) \cdots \alpha_k(d_k)$ and symbolic suffix $w = \alpha_{k+1} \cdots \alpha_{k+n}$

Result: A characteristic predicate for $u$ and $w$ in $\mathcal{M}$

1. $G := \top$, $H := \bot$, $V := \{x_1, \ldots, x_{k+n}\}$
2. while $\exists$ valuation $\nu$ for $V$ that extends $\nu_u$ such that $\nu \models G$ do
3.   $\nu := $ valuation for $V$ that extends $\nu_u$ such that $\nu \models G$
4.   $z := \alpha_1(\nu(x_1)) \cdots \alpha_{k+n}(\nu(x_{k+n}))$ // Construct membership query
5.   $I := \bigwedge_{i=k+1}^{k+n} \text{constraints}_\mathcal{M}(z)[i]$ // Constraints resulting from query
6. if $z \in L(\mathcal{M})$ then // Result query 'yes' or 'no'
7.   $H := H \lor I$
8. $G := G \land \neg I$
9. end
10. return $H$

that is, $H$ characterizes the data words $u'$ with $\text{Acts}(u') = w$ such that $u \cdot u'$ is accepted by $\mathcal{M}$. In the case of the FIFO-buffer example from Figure 2, a characteristic predicate for prefix $\text{Push}(5) \text{Push}(7)$ and symbolic suffix $\text{Pop Pop}$ is $x_3 = x_1 \land x_4 = x_2$. A characteristic predicate for the empty prefix and symbolic suffix $\text{Pop}$ is $\bot$, since this trace will inevitably lead to the sink location $l_3$ and there are no accepting words.

Algorithm 1 shows how a characteristic predicate may be computed by systematically exploring all the (finitely many) paths of $\mathcal{M}$ with prefix $u$ and suffix $w$ using tainted membership queries. During the execution of Algorithm 1, predicate $G$ describes the part of the parameter space that still needs to be explored, whereas $H$ is the characteristic predicate for the part of the parameter space that has been covered. We use the notation $H \equiv T$ to indicate syntactic equivalence, and $H = T$ to indicate logical equivalence. Note, if there exists no parameter space to be explored (i.e., $w$ is empty) and $u \in L(\mathcal{M})$, the algorithm returns $H \equiv \bot \lor T$ (as the empty conjunction equals $\top$).

Example 6 (Algorithm 1). Consider the FIFO-buffer example and the tree query with prefix $\text{Push}(5) \text{Push}(7)$ and symbolic suffix $\text{Pop Pop}$. After the prefix location $l_2$ is reached. From there, three paths are possible with actions $\text{Pop Pop}$: $l_2l_3l_3$, $l_2l_1l_3$, and $l_2l_1l_0$. We consider an example run of Algorithm 1.

Initially, $G_0 \equiv T$ and $H_0 \equiv \bot$. Let $\nu_1 = [x_1 \mapsto 5, x_2 \mapsto 7, x_3 \mapsto 1, x_4 \mapsto 1]$. Then $\nu_1$ extends $\nu_u$ and $\nu_1 \models G_0$. The resulting tainted run corresponds to path $l_2l_3l_3$ and so the tainted query gives path constraint $I_1 \equiv x_3 \neq x_1 \land \top$. Since the tainted run is rejecting, $H_1 \equiv \bot$ and $G_1 \equiv \top \land \neg I_1$.

In the next iteration, we set $\nu_2 = [x_1 \mapsto 5, x_2 \mapsto 7, x_3 \mapsto 5, x_4 \mapsto 1]$. Then $\nu_2$ extends $\nu_u$ and $\nu_2 \models G_1$. The resulting tainted run corresponds to path $l_2l_1l_3$ and so the tainted query gives path constraint $I_2 \equiv x_3 = x_1 \land x_4 \neq x_2$. Since the tainted run is rejecting, $H_2 \equiv \bot$ and $G_2 \equiv \top \land \neg I_1 \land \neg I_2$.

In the final iteration, we set $\nu_3 = [x_1 \mapsto 5, x_2 \mapsto 7, x_3 \mapsto 5, x_4 \mapsto 7]$. Then $\nu_3$ extends $\nu_u$ and $\nu_3 \models G_2$. The resulting tainted run corresponds to path $l_2l_1l_0$. 

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and the tainted query gives path constraint $I_3 \equiv x_3 = x_1 \land x_4 = x_2$. Now the tainted run is accepting, so $H_3 \equiv \bot \lor I_3$ and $G_3 = \top \land \neg I_1 \land \neg I_2 \land \neg I_3$. As $G_3$ is unsatisfiable, the algorithm terminates and returns characteristic predicate $H_3$.

**Construction of a non-minimal SDT** For each tree query with prefix $u$ and symbolic suffix $w$, the corresponding characteristic predicate $H$ is sufficient to construct an SDT using Algorithm 2.

**Algorithm 2: SDTConstructor**

| Data: Characteristic predicate $H$, index $n = k + 1$, Number of suffix parameters $N$ |
|-----------------------------------------------------------|
| Number of suffix parameters $N$ |
| Result: Non-minimal SDT $T$ |

1. if $n = k + N + 1$ then
   2. $l_0 :=$ SDT node
   3. $z :=$ if $H \iff \bot$ then $-$ else + // Value $\lambda$ for leaf node of the SDT
   4. return $\langle \{ l_0 \}, l_0, [l_0 \mapsto \emptyset], \emptyset, [l_0 \mapsto z] \rangle$ // RA with single location

5. else
   6. $T :=$ SDT node
   7. $I_t := \{ i \mid x_n \odot x_i \in H, n > i \}$ // $x_i$ may be a parameter or a constant
   8. if $I_t$ is $\emptyset$ then
      9. $t :=$ SDTConstructor($H, n + 1, N$) // No guards present
     10. Add $t$ with guard $\top$ to $T$
   11. else
      12. $g := \bigwedge_{i \in I_t} x_n \neq x_i$ // Disequality guard case
     13. $H' := \bigvee_{f \in H} f \land g$ if $f \land g$ is satisfiable else $\bot$ // $f$ is a disjunct
     14. $t' :=$ SDTConstructor($H', n + 1, N$)
     15. Add $t'$ with guard $g$ to $T$
   16. for $i \in I_t$ do
      17. $g := x_n = x_i$ // Equality guard case
     18. $H' := \bigvee_{f \in H} f \land g$ if $f \land g$ is satisfiable else $\bot$
     19. $t' :=$ SDTConstructor($H', n + 1, N$)
     20. Add $t'$ with guard $g$ to $T$
   21. end
   22. return $T$

Algorithm 2 proceeds in the following manner: for a symbolic action $\alpha(x_n)$ with parameter $x_n$, construct the potential set $I_t$ (lines 6 & 7), that is, the set of parameters to which $x_n$ is compared to in $H$. For line 7, recall that $H$ is a DNF formula, hence each literal $x_j \odot x_k$ is considered in the set comprehension, rather than the conjunctions making up the predicate $H$. Each element $x_i \in I_t$ can be either a formal parameter in the tree query or a constant $c_i \in C$ from our chosen structure. Using $I_t$, we can construct the guards as follows:

- **Disequality guard**: The disequality guard will be $g := \bigwedge_{i \in I_t} x_n \neq x_i$.

We can then check which guards in $H$ are still satisfiable with the addition
of $g$ and constructs the predicate $H'$ for the next call of Algorithm 2 (lines 13–16).

- **Equality guard** ($s$): For each parameter $x_i$ for $i \in I_t$, the equality guard will be $g := x_n = x_i$. We can then check which guards in $H$ are still satisfiable with the addition of $g$ and this becomes the predicate $H'$ for the next call of Algorithm 2 (lines 18–21).

At the base case (lines 1–4), there are no more parameters remaining and we return a non-accepting leaf if $H = \bot$, otherwise accepting. As mentioned, at each non-leaf location $l$ of the SDT $T$ returned by Algorithm 2, there exists a potential set $I_l$. For each parameter $x_i$, we know that there is a comparison between $x_i$ and $x_n$ in the SUT.

**Example 7 (Algorithm 2).** Consider a characteristic predicate $H \equiv I_1 \lor I_3 \lor I_4$, where $I_1 \equiv x_2 \neq x_1 \land x_3 \neq x_1$, $I_2 \equiv x_2 = x_1 \land x_3 \neq x_1$, $I_3 \equiv x_2 \neq x_1 \land x_3 = x_1$, $I_4 \equiv x_2 = x_1 \land x_3 = x_1$. We discuss only the construction of the sub-tree rooted at node $s_{21}$ for the SDT visualised in Figure 4a; the construction of the remainder is similar.

Initially, $x_n = x_{k+1} = x_2$. Potential set $I_t$ for $x_2$ is $\{x_1\}$ as $H$ contains the literals $x_2 = x_1$ and $x_2 \neq x_1$. Consider the construction of the equality guard $g := x_2 = x_1$. The new characteristic predicate is $H' \equiv (I_2 \land g) \lor (I_4 \land g)$, as $I_1$ and $I_3$ are unsatisfiable when conjugated with $g$.

For the next call, with $n = 3$, the current variable is $x_3$, with predicate $H = H'$ (from the parent instance). We obtain the potential set for $x_3$ as $\{x_1\}$. The equality guard is $g' := x_3 = x_1$ with the new characteristic predicate $H'' \equiv I_4 \land g \land g'$, i.e., $H'' \iff x_2 = x_1 \land x_3 = x_1$ (note, $I_2 \land g \land g'$ is unsatisfiable). In the next call, we have $n = 4$, thus we compute a leaf. As $H''$ is not $\bot$, we return an accepting leaf $t$. The disequality guard is $g'' := x_3 \neq x_1$ with characteristic predicate $H''' \iff x_2 = x_1 \land x_3 = x_1 \land x_3 \neq x_1 \iff \bot$. In the next call, we have $n = 4$, and we return a non-accepting leaf $t'$. The two trees $t$ and $t'$ are added as sub-trees with their respective guards $g'$ and $g''$ to a new tree rooted at node $s_{21}$ (see Figure 4a).

**SDT Minimisation** Example 7 showed a characteristic predicate $H$ containing redundant comparisons, resulting in the non-minimal SDT in Figure 4a. We use Algorithm 3 to minimise the SDT in Figure 4a to the SDT in Figure 4b.

We present an example of the application of Algorithm 3, shown for the SDT of Figure 4a. Figure 4a visualises a non-minimal SDT $T$, where $s_{20}$ and $s_{21}$ (in red) are essentially “duplicates” of each other: the sub-tree for node $s_{20}$ is isomorphic to the sub-tree for node $s_{21}$ under the relabelling “$x_2 = x_1$”. We indicate this relabelling using the notation $T[s_{20}]\langle x_1, x_2 \rangle$ and the isomorphism relation under the relabelling as $T[s_{20}]\langle x_1, x_2 \rangle \simeq T[s_{21}]$. Algorithm 3 accepts the non-minimal SDT of Figure 4a and produces the equivalent minimal SDT in Figure 4b. Nodes $s_{20}$ and $s_{21}$ are merged into one node, $s_2$, marked in green. We can observe that both SDTs still encode the same decision tree. With Algorithm 3, we have completed our tainted tree oracle, and can now proceed to the tainted equivalence oracle.
Algorithm 3: MinimiseSDT

Data: Non-minimal SDT $T$, current index $n$
Result: Minimal SDT $T'$

1. if $T$ is a leaf then // Base case
2. return $T$
3. else
4. $T' :=$ SDT node
5. // Minimise the lower levels
6. for guard $g$ with associated sub-tree $t$ in $T$ do
7. Add guard $g$ with associated sub-tree MinimiseSDT($t, n + 1$) to $T'$
8. end
9. // Minimise the current level
10. $I :=$ Potential set of root node of $T$
11. $t' :=$ disequality sub-tree of $T$ with guard $\bigwedge_{i \in I} x_n \neq x_i$
12. $I' := \emptyset$
13. for $i \in I$ do
14. if $t'(x_i, x_n) \neq t$ or $t'(x_i, x_n)$ is undefined then
15. $I' := I' \cup \{x_i\}$
16. Add guard $x_n = x_i$ with corresponding sub-tree $t$ to $T'$
17. end
18. Add guard $\bigwedge_{i \in I'} x_n \neq x_i$ with corresponding sub-tree $t'$ to $T'$
19. return $T'$

4.2 Tainted Equivalence Oracle

The tainted equivalence oracle (TEO), similar to its non-tainted counterpart, accepts a hypothesis $H$ and verifies whether $H$ is equivalent to register automaton $M$ that models the SUT. If $H$ and $M$ are equivalent, the oracle replies “yes”, otherwise it returns “no” together with a CE. The RandomWalk Equivalence Oracle in RALib constructs random traces in order to find a CE.

Definition 4 (Tainted Equivalence Oracle). For a given hypothesis $H$, maximum word length $n$, and an SUT $S$, a tainted equivalence oracle is a function $O_E(H, n, S)$ for all tainted traces $w$ of $S$ where $|w| \leq n$, $O_E(H, n, S)$ returns $w$ if $w \in \mathcal{L}(H) \iff w \in \mathcal{L}(S)$ is false, and ‘Yes’ otherwise.

The TEO is similar to the construction of the characteristic predicate to find a CE: we randomly generate a symbolic suffix of specified length $n$ (with an empty prefix), and construct a predicate $H$ for the query. For each trace $w$ satisfying a guard in $H$, we confirm whether $w \in \mathcal{L}(H) \iff w \in \mathcal{L}(M)$. If false, $w$ is a CE. If no $w$ is false, then we randomly generate another symbolic suffix. In practice, we bound the number of symbolic suffixes to generate. Example 8 presents a scenario of a combination lock automaton that can be learned (relatively easily) using a TEO but cannot be handled by normal oracles.

Example 8 (Combination Lock RA). A combination lock is a type of RA which requires a sequence of specific inputs to ‘unlock’. Figure 5 presents an RA $C$...
with a ‘4-digit’ combination lock that can be unlocked by the sequence \( w = \alpha(c_0)\alpha(c_1)\alpha(c_2)\alpha(c_3) \), where \( \{c_0, c_1, c_2, c_3\} \) are constants. Consider a case where a hypothesis \( \mathcal{H} \) is being checked for equivalence against the RA \( \mathcal{C} \) with \( w \not\in L(\mathcal{H}) \). While it would be difficult for a normal equivalence oracle to generate the word \( w \) randomly; the tainted equivalence oracle will record at every location the comparison of input data value \( p \) with some constant \( c_i \) and explore all corresponding guards at the location, eventually constructing the word \( w \).

For the combination lock automaton, we may note that as the ‘depth’ of the lock increases, the possibility of randomly finding a CE decreases.

5 Experimental Evaluation

We have used stubbed versions of the Python FIFO-Queue and Set modules\(^5\) for learning the FIFO and Set models, while the Combination Lock automata were constructed manually. Source code for all other models was obtained by

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\(^5\) From Python’s \texttt{queue} module and standard library, respectively.
translating existing benchmarks from [18] (see also automata.cs.ru.nl) to Python code. We also utilise a ‘reset’ operation: A ‘reset’ operation brings an SUT back to its initial state, and is counted as an ‘input’ for our purposes. Furthermore, each experiment was repeated 30 times with different random seeds. Each experiment was bounded according to the following constraints: learning phase: $10^9$ inputs and $5 \times 10^7$ resets; testing phase: $10^9$ inputs and $5 \times 10^4$ resets; length of the longest word during testing: 50; and a ten-minute timeout for the learner to respond.

Figure 6 gives an overview of our experimental results. We use the notation ‘TTO’ to represent ‘Tainted Tree Oracle’ (with similar labels for the other oracles). In the figure, we can see that as the size of the container increases, the difference between the fully tainted version (TTO+TEO, in blue) and the completely untainted version (NTO+NEO, in red) increases. In the case where only a tainted tree oracle is used (TTO+NEO, in green), we see that it is following the fully tainted version closely (for the FIFO models) and is slightly better in the case of the SET models.

Fig. 6: Benchmark plots: Number of symbols used with tainted oracles (blue and green) are generally lower than with normal oracles (red and orange). Note that the y-axis is log-scaled. Additionally, normal oracles are unable to learn the Combination Lock and Repetition automata and are hence not plotted.
The addition of the TEO gives a conclusive advantage for the Combination Lock and Repetition benchmarks. The addition of the TTO by itself results in significantly fewer number of symbols, even without the tainted equivalence oracle (TTO v/s NTO, compare the green and red lines). With the exception of the Combination Lock and Repetition benchmarks, the TTO+TEO combination does not provide vastly better results in comparison to the TTO+NEO results, however, it is still (slightly) better. We note that — as expected — the NEO does not manage to provide CEs for the Repetition and Combination Lock automata. The TEO is therefore much more useful for finding CEs in SUTs which utilise constants. For complete details of the data used to produce the plots, please refer to Appendix B.

6 Conclusions and Future Work

In this article, we have presented an integration of dynamic taint analysis, a white-box technique for tracing data flow, and register automata learning, a black-box technique for inferring behavioral models of components. The combination of the two methods improves upon the state-of-the-art in terms of class of systems for which models can be generated and in terms of performance: Tainting makes it possible to infer data-flow constraints even in instances with a high essential complexity (e.g., in the case of so-called combination locks). Our implementation outperforms pure black-box learning by two orders of magnitude with a growing impact in the presence of multiple data parameters and registers. Both improvements are important steps towards the applicability of model learning in practice as they will help scaling to industrial use cases.

At the same time our evaluation shows the need for further improvements: Currently, the SL∗ algorithm uses symbolic decision trees and tree queries globally, a well-understood weakness of learning algorithms that are based on observation tables. It also uses individual tree oracles each type of operation and relies on syntactic equivalence of decision trees. A more advanced learning algorithm for extended finite state machines will be able to consume fewer tree queries, leverage semantic equivalence of decision trees. Deeper integration with white-box techniques could enable the analysis of many (and more involved) operations on data values.

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Appendix A  Tree Oracle for Equalities

In this appendix, we prove that the tainted tree oracle generates SDTs which are isomorphic to the SDTs generated by the normal tree oracle as defined in [6]. In order to do so, we first introduce the constructs used by Cassel et al. [6] for generating SDTs. We begin with some preliminaries:

For a word $u$ with $\text{Vals}(u) = d_1 \ldots d_k$, we define a potential of $u$. The potential of $u$, written as $\text{pot}(u)$, is the set of indices $i \in \{1, \ldots, k\}$ for which there exists no $j \in \{1, \ldots, k\}$ such that $j > i$ and $d_i = d_j$. The concept of potential essentially allows unique access to a data value, abstracting away from the concrete position of a data value in a word. For a guard $g$ defined over $\mathcal{V}^+$ for a word $u$ with $\text{Vals}(u) = d_1 \ldots d_k$, a representative data value $d_u^2$ is a data value s.t. $\nu(u) \cup \{[p \mapsto d_u^2]\} = g$. Furthermore, for a word $w = \alpha \cdot w'$ (where $w'$ may be $\epsilon$), $w'$ can be represented as $\alpha^{-1}w$. The same notation is also extended to sets of words: $\alpha^{-1}V = \{\alpha^{-1}w \mid w \in V\}$.

We may now define an SDT:

Definition 5 (Symbolic Decision Tree). A Symbolic Decision Tree (SDT) is a register automaton $T = (L, l_0, X, \Gamma, \lambda)$ where $L$ and $\Gamma$ form a tree rooted at $l_0$.

For location $l$ of SDT $T$, we write $T[l]$ to denote the subtree of $T$ rooted at $l$. An SDT that results from a tree query $(u, w)$ (of a prefix word $u$ and a symbolic suffix $w$), is required to satisfy some canonical form, captured by the following definition.

Definition 6 ($(u, w)$-tree). For any data word $u$ with $k$ actions and any symbolic suffix $w$, a $(u, w)$-tree is an SDT $T$ which has runs over all data words in $[u]$, and which satisfies the following restriction: whenever $(l, \alpha(p), g, \pi, l')$ is the $j^{th}$ transition on some path from $l_0$, then for each $x_i \in X(l')$ we have either (i) $i < k + j$ and $\pi(x_i) = x_i$, or (ii) $i = k + j$ and $\pi(x_i) = p$.

If $u = \alpha(d_1) \cdots \alpha_k(d_k)$ is a data word then $\nu_u$ is the valuation of $\{x_1, \ldots, x_k\}$ satisfying $\nu_u(x_i) = d_i$, for $1 \leq i \leq k$. Using this definition, the notion of a tree oracle, which accepts tree queries and returns SDTs, can be described as follows.

Definition 7 (Tree Oracle). A tree oracle for a structure $S$ is a function $\mathcal{O}$ which, for a data language $\mathcal{L}$, prefix word $u$ and symbolic suffix $w$ returns a $(u, w)$-tree $\mathcal{O}(\mathcal{L}, u, w)$ s.t. for any word $v \in [u]$, the following holds: $v$ is accepted by $\mathcal{O}(\mathcal{L}, u, w)$ under $\nu_u$ iff $u \cdot v \in \mathcal{L}$.

A tree oracle returns equality trees, defined below:

Definition 8 (Equality Tree). An equality tree for a tree query $(u, V)$ is a $(u, V)$-tree $T$ such that:

- for each action $\alpha$, there is a potential set $I \subseteq \text{pot}(u)$ of indices such that the initial $\alpha$-guards consist of the equalities of form $p = x_i$ for $i \in I$ and one disequality of form $\wedge_{i \in I} p \neq x_i$, and
– for each initial transition \((l_0, \alpha(p), g, l)\) of \(T\), the tree \(T[l]\) is an equality tree for \((u\alpha(d^0), \alpha^{-1}V)\).

Cassel et al. [6] require their (equality trees) SDTs to be minimal (called maximally abstract in [6]), i.e., the SDTs must not contain any redundancies (such as Figure 4a). This can be achieved by checking if two sub-trees are equal under some relabelling, and the process of constructing a tree by relabelling an equality sub-tree is called specialisation of equality tree:

**Definition 9 (Specialisation of equality tree).** Let \(T\) be an equality tree for prefix \(u\) and set of symbolic suffixes \(V\), and let \(J \subseteq \text{pot}(u)\) be a set of indices. Then \(T(J)\) denotes the equality tree for \((u, V)\) obtained from \(T\) by performing the following transformations for each \(\alpha\):

- Whenever \(T\) has several initial \(\alpha\)-transitions of form \((l_0, \alpha(p), (p = x_j), l_j)\) with \(j \in J\), then all subtrees of form \((T[l_j])(J[(k + 1) \mapsto j])\) for \(j \in J\) must be defined and isomorphic, otherwise \(T(J)\) is undefined. If all such subtrees are defined and isomorphic, then \(T(J)\) is obtained from \(T\) by
  1. replacing all initial \(\alpha\)-transitions of form \((l_0, \alpha(p), (p = x_j), l_j)\) for \(j \in J\) by the single transition \((l_0, \alpha(p), (p = x_m), l_m)\) where \(m = \max(J)\),
  2. replacing \(T[l_m]\) by \((T[l_m])(J[(k + 1) \mapsto m])\), and
  3. replacing all other subtrees \(T[l']\) reached by initial \(\alpha\)-transitions (which have not been replaced in Step 1) by \((T[l'])(J)\).

If, for some \(\alpha\), any of the subtrees generated in Step 2 or 3 are undefined, then \(T(J)\) is also undefined, otherwise \(T(J)\) is obtained after performing Steps 1 – 3 for each \(\alpha\).

**Definition 10 (Necessary Potential set for Tree Oracle).** A necessary potential set \(I\) for the root location \(l_0\) of an equality tree \(O(L, u, V)\) is a subset of \(\text{pot}(u)\) such that for each index \(i \in I\) the following holds:

1. \(O(L, u\alpha(d^0_i), V_\alpha)(\{i, k + 1\})\) is undefined, or
2. \(O(L, u\alpha(d^0_i), V_\alpha)(\{i, k + 1\}) \neq O(L, u\alpha(d_i), V_\alpha)\).

Intuitively, a necessary potential set contains indices of data values which influence future behaviour of the SUT. Consequently, indices of data values which do not influence the behaviour of the SUT are excluded from the necessary potential set. We are now ready to define the tree oracle for equality:

**Definition 11 (Tree oracle for equality).** For a language \(L\), a prefix \(u\), and the set of symbolic suffixes \(V\), the equality tree \(O(L, u, V)\) is constructed as follows:

- If \(V = \{\epsilon\}\), then \(O(L, u, \{\epsilon\})\) is the trivial tree with one location \(l_0\) and no registers. It is accepting if the word is accepted, i.e., \(\lambda(l_0) = +\) if \(u \in L\), else \(\lambda(l_0) = -.\) To determine \(u \in L\), the tree oracle performs a membership query on \(u\).
- If \(V \neq \{\epsilon\}\), then for each \(\alpha\) such that \(V_\alpha = \alpha^{-1}V\) is non-empty,
We recall that, under the test hypothesis, an SUT $\mathcal{M}$ is deterministic and has a finite number of logically disjoint branches to be followed from each state.

Algorithm 1 initialises two variables $G := \top$ and $H := \bot$. For each word $z = u \cdot w$ under a valuation $\nu \models G$, we may perform a membership query on $\mathcal{M}$. Each query returns the guard $I = \bigwedge_{i=k+1}^{k+n+1} \text{constraints}_{\mathcal{M}}(z)[i]$ such that $\nu \models I$ and the acceptance of the word $z$ in the language of $\mathcal{M}$, i.e., $z \in \mathcal{L}$. 

### Lemma 1 (Characteristic Predicate)

For a tree query $(u, w)$, Algorithm 1 always produces a characteristic predicate $H$. 

**Proof.** We recall that, under the test hypothesis, an SUT $\mathcal{M}$ is deterministic and has a finite number of logically disjoint branches to be followed from each state. Algorithm 1 initialises two variables $G := \top$ and $H := \bot$. For each word $z = u \cdot w$ under a valuation $\nu \models G$, we may perform a membership query on $\mathcal{M}$. Each query returns the guard $I = \bigwedge_{i=k+1}^{k+n+1} \text{constraints}_{\mathcal{M}}(z)[i]$ such that $\nu \models I$ and the acceptance of the word $z$ in the language of $\mathcal{M}$, i.e., $z \in \mathcal{L}$. 

Intuitively, $\mathcal{O}(\mathcal{L}, u, V)$ is constructed by joining the trees $\mathcal{O}(\mathcal{L}, \nu \alpha(d_i), V)$ with guard $p = x_i$ for $i \in I$, and the tree $\mathcal{O}(\mathcal{L}, \nu \alpha(d_0), V)$ with guard $\bigwedge_{i \in I} p \neq x_i$, as children of a new root. Note, while $V$ is a set of symbolic suffixes, RALib technically handles tree queries sequentially, i.e., as sequential tree queries of prefix $u$ and symbolic suffix $w$. Consequently, we treat the set of symbolic suffixes $V$ as a singleton, referred to as ‘$w$’.

$\mathcal{O}(\mathcal{L}, u, w)$ is constructed bottom-up, recursively building new ‘roots’ at the top with larger and larger symbolic suffixes (and consequently, shorter and shorter prefixes). The choice of the necessary potential set $I$ plays a crucial role: if $I$ is larger than necessary, $\mathcal{O}(\mathcal{L}, u, w)$ contains redundant guards (and is hence a ‘non-minimal’ SDT).

We now have a clear goal for our proof: we must show that the SDT returned by Algorithm 3 is isomorphic to the SDT returned by the tree oracle for equality as defined in Definition 11 (under the assumption that the ‘set’ of symbolic suffixes $V$ is a singleton). We can divide our proof into the following steps:

1. We show that Algorithm 1 produces a characteristic predicate for tree query $(u, w)$, and contains all the information for constructing an equality tree.
2. Next, we show that Algorithm 2 guarantees that for potential set $I_i$ of a location $l_i$ of the tainted equality tree $T_i$, the potential set $I$ of equivalent location $l$ of the normal equality tree $T$ is a subset of $I_i$: $I \subseteq I_i$, and finally,
3. We can then reduce the make the tainted potential set equal to the normal potential set (using Algorithm 3) and the resulting tainted equality tree will be isomorphic to the normal equality tree.

Each of the above steps correspond to one of our algorithms. We now begin with step 1: from Algorithm 1, we can state the following lemmas:

### Lemma 1 (Characteristic Predicate) For a tree query $(u, w)$, Algorithm 1 always produces a characteristic predicate $H$.

**Proof.** We recall that, under the test hypothesis, an SUT $\mathcal{M}$ is deterministic and has a finite number of logically disjoint branches to be followed from each state. Algorithm 1 initialises two variables $G := \top$ and $H := \bot$. For each word $z = u \cdot w$ under a valuation $\nu \models G$, we may perform a membership query on $\mathcal{M}$. Each query returns the guard $I = \bigwedge_{i=k+1}^{k+n+1} \text{constraints}_{\mathcal{M}}(z)[i]$ such that $\nu \models I$ and the acceptance of the word $z$ in the language of $\mathcal{M}$, i.e., $z \in \mathcal{L}$. 

...
For each iteration of the do-while loop, the variable $G$ is updated with the negation of the previously-satisfied guard $I$, i.e., $G := G \land \neg I$. This guarantees that any new valuation $\nu'$ will not satisfy $I$, and hence, the next iteration of the do-while loop shall induce a different run of $M$. Given that $M$ only has a finite number of logical branches, Algorithm 1 terminates.

We also know that for each tainted word $z$, we obtain the acceptance of $z \in L(M)$. If $z \in L(M)$, the variable $H$ is updated to $H \lor I$. Therefore, the predicate $H$ returned by Algorithm 1 is the characteristic predicate for the tree query $(u, w)$.

After constructing the characteristic predicate, we convert it to a non-minimal SDT using Algorithm 2, providing us with the following lemma:

**Lemma 2 (Non-minimal SDT).** For any location $l_t$ of a non-minimal SDT with an equivalent location $l$ of a minimal SDT, the necessary potential set $I_t$ of the non-minimal SDT is a superset of the necessary potential set $I$ of the minimal SDT: $I \subseteq I_t \subseteq \text{pot}(u)$ where $\text{pot}(u)$ is the potential of the prefix $u$ of locations $l_t$ and $l$.

**Proof.** We know that $I \subseteq \text{pot}(u)$ by definition of the necessary potential set. For any word $w = u \cdot v$ where the prefix $u$ leads to location $l_t$ of the tainted non-minimal SDT, Algorithm 2 guarantees that the suffixes of $u$ will be classified correctly. If the suffixes are classified correctly, we derive that $I_t \supseteq I$ (otherwise the suffixes will not be classified correctly). Since $I_t \supseteq I$ and $I, I_t \subseteq \text{pot}(u)$, we conclude $I \subseteq I_t \subseteq \text{pot}(u)$. \hfill $\Box$

Following Lemma 2, if we wish to make $I = I_t$, we can simply remove all elements from $I_t$ which do not satisfy the conditions outlined in Definition 10. Since we already know that $I \subseteq I_t$, we can confirm that after removal of all irrelevant parameters, $I = I_t$. Algorithm 3 accomplishes the same.

Cassel et al. [6] use the concept of representative data values for constructing the SDT, while we treat the values symbolically: a representative data value ‘represents’ the set of data values that satisfy a guard during construction of the SDT; in our case, we simply let $Z_3$ decide on all the values to use for our membership queries and obtain the guards about them using their taint markers as identifiers.

**Theorem 1 (Isomorphism of tree oracles).** The SDTs generated by the tainted tree oracle and the untainted tree oracle for a tree query $(u, w)$ are isomorphic.

**Proof.** Lemma 1 guarantees that Algorithm 1 returns a characteristic predicate $H$ for the tree query $(u, w)$. Application of Algorithm 2 on $H$ constructs a non-minimal SDT. Using Lemma 2 and Algorithm 3 on the non-minimal SDT, we can conclude that the root locations of the tainted tree oracle and normal tree oracle have the same necessary potential set. By inductive reasoning on the depth of the trees, the same holds for all sub-trees of both oracles, eventually reducing to the leaves, showing that the tainted tree oracle is isomorphic to tree oracle. \hfill $\Box$
## Appendix B  Detailed Benchmark results

Table 1 contains the full results of the values used to create the plots from Figure 6.

**Table 1: Benchmarks**

| Model          | Tree Oracle | EQ Oracle | Learn Symbols | Test Symbols | Total Symbols Learned |
|----------------|-------------|-----------|---------------|--------------|-----------------------|
|                |             |           | (Std. Dev)    | (Std. Dev)   | (Std. Dev)            |
| Abp Output     | Tainted     | Normal    | 6.55E+02      | 1.57E+05     | 1.58E+05              | 30/30                |
|                |             |           | (8.33E+01)    | (1.29E+05)   | (1.29E+05)            |                       |
| Abp Output     | Tainted     | Tainted   | 6.17E+02      | 1.68E+04     | 1.74E+04              | 30/30                |
|                |             |           | (7.78E+01)    | (1.15E+04)   | (1.15E+04)            |                       |
| Abp Output     | Normal      | Normal    | 6.93E+03      | 1.57E+05     | 1.64E+05              | 30/30                |
|                |             |           | (5.20E+03)    | (1.29E+05)   | (1.29E+05)            |                       |
| Abp Output     | Normal      | Tainted   | 6.51E+03      | 1.68E+04     | 2.33E+04              | 30/30                |
|                |             |           | (3.97E+03)    | (1.15E+04)   | (1.29E+04)            |                       |
| Lock 2         | Tainted     | Normal    | N-A           | N-A          | N-A                   | 0/30                  |
|                |             |           | (N-A)         | (N-A)        | (N-A)                 |                       |
| Lock 2         | Tainted     | Tainted   | 7.10E+01      | 1.15E+03     | 1.22E+03              | 30/30                |
|                |             |           | (0.00E+00)    | (6.76E+02)   | (6.76E+02)            |                       |
| Lock 2         | Normal      | Normal    | N-A           | N-A          | N-A                   | 0/30                  |
|                |             |           | (N-A)         | (N-A)        | (N-A)                 |                       |
| Lock 2         | Normal      | Tainted   | 2.00E+02      | 1.15E+03     | 1.35E+03              | 30/30                |
|                |             |           | (0.00E+00)    | (6.76E+02)   | (6.76E+02)            |                       |
| Lock 4         | Tainted     | Normal    | N-A           | N-A          | N-A                   | 0/30                  |
|                |             |           | (N-A)         | (N-A)        | (N-A)                 |                       |
| Lock 4         | Tainted     | Tainted   | 2.41E+02      | 6.29E+03     | 6.53E+03              | 30/30                |
|                |             |           | (0.00E+00)    | (5.52E+03)   | (5.52E+03)            |                       |
| Lock 4         | Normal      | Normal    | N-A           | N-A          | N-A                   | 0/30                  |
|                |             |           | (N-A)         | (N-A)        | (N-A)                 |                       |
| Lock 4         | Normal      | Tainted   | 3.45E+04      | 6.29E+03     | 4.08E+04              | 30/30                |
|                |             |           | (0.00E+00)    | (5.52E+03)   | (5.52E+03)            |                       |
| Lock 5         | Tainted     | Normal    | N-A           | N-A          | N-A                   | 0/30                  |
|                |             |           | (N-A)         | (N-A)        | (N-A)                 |                       |
| Lock 5         | Tainted     | Tainted   | 3.80E+02      | 2.62E+04     | 2.66E+04              | 30/30                |
|                |             |           | (0.00E+00)    | (1.45E+04)   | (1.45E+04)            |                       |
| Lock 5         | Normal      | Normal    | N-A           | N-A          | N-A                   | 0/30                  |
|                |             |           | (N-A)         | (N-A)        | (N-A)                 |                       |
| Lock 5         | Normal      | Tainted   | 6.35E+05      | 2.62E+04     | 6.61E+05              | 30/30                |
|                |             |           | (0.00E+00)    | (1.45E+04)   | (1.45E+04)            |                       |

Continued on next page
## Table 1: Benchmarks

| Model | Tree Oracle | EQ Oracle | Learn Symbols (Std. Dev) | Test Symbols (Std. Dev) | Total Symbols (Std. Dev) | Learned |
|-------|-------------|-----------|--------------------------|-------------------------|--------------------------|---------|
| Fifo 01 | Tainted | Taint | 2.90E+01 *(4.08E+00)* | 1.71E+01 *(6.12E+00)* | 4.62E+01 *(6.73E+00)* | 30/30 |
| Fifo 01 | Tainted | Tainted | 2.97E+01 *(3.83E+00)* | 1.38E+01 *(3.58E+00)* | 4.35E+01 *(4.93E+00)* | 30/30 |
| Fifo 01 | Normal | Normal | 6.65E+01 *(1.84E+01)* | 1.71E+01 *(6.12E+00)* | 8.37E+01 *(1.80E+01)* | 30/30 |
| Fifo 01 | Normal | Tainted | 7.07E+01 *(1.74E+01)* | 1.38E+01 *(3.58E+00)* | 8.46E+01 *(1.68E+01)* | 30/30 |
| Fifo 02 | Tainted | Normal | 1.16E+02 *(3.26E+01)* | 6.47E+01 *(2.77E+01)* | 1.81E+02 *(4.28E+01)* | 30/30 |
| Fifo 02 | Tainted | Tainted | 1.01E+02 *(3.03E+01)* | 5.10E+01 *(1.55E+01)* | 1.52E+02 *(3.31E+01)* | 30/30 |
| Fifo 02 | Normal | Normal | 3.62E+02 *(1.29E+02)* | 6.47E+01 *(2.77E+01)* | 4.27E+02 *(1.33E+02)* | 30/30 |
| Fifo 02 | Normal | Tainted | 3.50E+02 *(1.48E+02)* | 5.10E+01 *(1.55E+01)* | 4.01E+02 *(1.49E+02)* | 30/30 |
| Fifo 03 | Tainted | Normal | 3.03E+02 *(8.53E+01)* | 1.34E+02 *(5.84E+01)* | 4.38E+02 *(9.39E+01)* | 30/30 |
| Fifo 03 | Tainted | Tainted | 2.93E+02 *(8.54E+01)* | 1.05E+02 *(4.69E+01)* | 3.98E+02 *(8.07E+01)* | 30/30 |
| Fifo 03 | Normal | Normal | 1.64E+03 *(9.00E+02)* | 1.34E+02 *(5.84E+01)* | 1.78E+03 *(8.82E+02)* | 30/30 |
| Fifo 03 | Normal | Tainted | 1.93E+03 *(1.34E+03)* | 1.05E+02 *(4.69E+01)* | 2.03E+03 *(1.31E+03)* | 30/30 |
| Fifo 04 | Tainted | Normal | 6.87E+02 *(1.51E+02)* | 2.20E+02 *(1.11E+02)* | 9.06E+02 *(2.14E+02)* | 30/30 |
| Fifo 04 | Tainted | Tainted | 6.35E+02 *(1.41E+02)* | 1.62E+02 *(7.53E+01)* | 7.96E+02 *(1.53E+02)* | 30/30 |
| Fifo 04 | Normal | Normal | 1.22E+04 *(1.22E+04)* | 2.20E+02 *(1.11E+02)* | 1.24E+04 *(1.22E+04)* | 30/30 |
| Fifo 04 | Normal | Tainted | 1.19E+04 *(1.21E+04)* | 1.62E+02 *(7.53E+01)* | 1.20E+04 *(1.21E+04)* | 30/30 |
| Fifo 05 | Tainted | Normal | 1.23E+03 *(3.35E+02)* | 3.53E+02 *(2.13E+02)* | 1.58E+03 *(4.49E+02)* | 30/30 |
| Fifo 05 | Tainted | Tainted | 1.32E+03 *(2.88E+02)* | 2.24E+02 *(9.79E+01)* | 1.54E+03 *(3.14E+02)* | 29/30 |
| Fifo 05 | Normal | Normal | 1.00E+05 *(1.00E+05)* | 3.19E+02 *(1.00E+05)* | 1.01E+05 *(25/30) | 25/30 |

Continued on next page
Table 1: Benchmarks

| Model | Tree Oracle | EQ Oracle | Learn Symbols | Test Symbols | Total Symbols | Total Symbols Learned |
|-------|-------------|-----------|---------------|--------------|---------------|-----------------------|
|       |             |           | (Std. Dev)    | (Std. Dev)   | (Std. Dev)    |                       |
| Fifo 05 | Normal      | Tainted   | 1.28E+05      | 2.35E+02     | 1.28E+05      | 25/30                |
|        |             |           | (2.08E+05)    | (8.76E+01)   | (2.08E+05)    |                       |
| Repetition | Tainted     | Normal    | N-A           | N-A          | N-A           | 0/30                  |
|         |             |           | (N-A)         | (N-A)        | (N-A)         |                       |
| Repetition | Tainted     | Tainted   | 1.22E+02      | 7.33E+03     | 7.45E+03      | 30/30                |
|         |             |           | (0.00E+00)    | (2.03E+03)   | (2.03E+03)    |                       |
| Repetition | Normal      | Normal    | N-A           | N-A          | N-A           | 0/30                  |
|         |             |           | (N-A)         | (N-A)        | (N-A)         |                       |
| Repetition | Normal      | Tainted   | 8.90E+03      | 7.33E+03     | 1.62E+04      | 30/30                |
|         |             |           | (1.99E+03)    | (2.03E+03)   | (2.06E+03)    |                       |
| Set 01  | Tainted     | Normal    | 1.45E+02      | 1.28E+03     | 1.43E+03      | 29/30                |
|         |             |           | (1.03E+02)    | (1.52E+03)   | (1.52E+03)    |                       |
| Set 01  | Tainted     | Tainted   | 9.75E+01      | 1.83E+02     | 2.80E+02      | 30/30                |
|         |             |           | (3.56E+01)    | (1.61E+02)   | (1.56E+02)    |                       |
| Set 01  | Normal      | Normal    | 5.00E+06      | 1.28E+03     | 5.01E+06      | 29/30                |
|         |             |           | (1.73E+07)    | (1.52E+03)   | (1.73E+07)    |                       |
| Set 01  | Normal      | Tainted   | 2.96E+03      | 1.83E+02     | 3.15E+03      | 30/30                |
|         |             |           | (6.71E+03)    | (1.61E+02)   | (6.69E+03)    |                       |
| Set 02  | Tainted     | Normal    | 1.61E+02      | 8.21E+03     | 9.82E+03      | 28/30                |
|         |             |           | (9.96E+02)    | (1.26E+04)   | (1.24E+04)    |                       |
| Set 02  | Tainted     | Tainted   | 1.00E+03      | 2.21E+02     | 1.23E+03      | 29/30                |
|         |             |           | (3.26E+02)    | (2.14E+02)   | (3.68E+02)    |                       |
| Set 02  | Normal      | Normal    | 4.61E+06      | 8.60E+03     | 4.62E+06      | 25/30                |
|         |             |           | (1.43E+07)    | (1.31E+04)   | (1.43E+07)    |                       |
| Set 02  | Normal      | Tainted   | 4.35E+04      | 2.20E+02     | 4.37E+04      | 30/30                |
|         |             |           | (7.28E+04)    | (2.10E+02)   | (7.29E+04)    |                       |
| Set 03  | Tainted     | Normal    | 1.76E+04      | 5.01E+03     | 2.26E+04      | 24/30                |
|         |             |           | (8.71E+03)    | (9.51E+03)   | (1.40E+04)    |                       |
| Set 03  | Tainted     | Tainted   | 1.44E+04      | 6.91E+02     | 1.51E+04      | 30/30                |
|         |             |           | (5.05E+03)    | (8.76E+02)   | (4.95E+03)    |                       |
| Set 03  | Normal      | Normal    | 5.76E+06      | 3.94E+03     | 5.76E+06      | 14/30                |
|         |             |           | (1.47E+07)    | (6.48E+03)   | (1.47E+07)    |                       |
| Set 03  | Normal      | Tainted   | 2.01E+06      | 2.23E+02     | 2.01E+06      | 28/30                |
|         |             |           | (3.60E+06)    | (2.06E+02)   | (3.60E+06)    |                       |
| Sip 2015| Tainted     | Normal    | 2.14E+03      | 1.89E+05     | 1.92E+05      | 10/30                |
|         |             |           | (4.00E+02)    | (2.60E+05)   | (2.60E+05)    |                       |
| Model      | Tree Oracle | EQ Oracle | Learn Symbols (Std. Dev) | Test Symbols (Std. Dev) | Total Symbols (Std. Dev) | Symbols Learned |
|------------|-------------|-----------|--------------------------|-------------------------|--------------------------|-----------------|
| Sip 2015   | Tainted     | Tainted   | 2.30E+03                 | 3.18E+04                | 3.41E+04                 | 29/30           |
|            |             |           | (3.13E+02)               | (1.59E+04)              | (1.59E+04)               |                 |
| Sip 2015   | Normal      | Normal    | 1.57E+05                 | 2.07E+05                | 3.65E+05                 | 9/30            |
|            |             |           | (4.42E+05)               | (2.69E+05)              | (4.81E+05)               |                 |
| Sip 2015   | Normal      | Tainted   | 1.47E+05                 | 3.18E+04                | 1.79E+05                 | 29/30           |
|            |             |           | (2.80E+05)               | (1.59E+04)              | (2.78E+05)               |                 |