A New Approach for Active Automata Learning Based on Apartness*

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Abstract. We present $L^\#$, a new and simple approach to active automata learning. Instead of focusing on equivalence of observations, like the L^* algorithm and its descendants, $L^\#$ takes a different perspective: it tries to establish *apartness*, a constructive form of inequality. $L^\#$ does not require auxiliary notions such as observation tables or discrimination trees, but operates directly on tree-shaped automata. $L^\#$ has the same asymptotic query and symbol complexities as the best existing learning algorithms, but we show that adaptive distinguishing sequences can be naturally integrated to boost the performance of $L^\#$ in practice. Experiments with a prototype implementation, written in Rust, suggest that $L^\#$ is competitive with existing algorithms.

Keywords: $L^\#$ algorithm · active automata learning · Mealy machine · apartness relation · adaptive distinguishing sequence · observation tree · conformance testing

1 Introduction

In 1987, Dana Angluin published a seminal paper [5], in which she showed that the class of regular languages can be learned efficiently using queries. In Angluin's approach of a *minimally adequate teacher (MAT)*, learning is viewed as a game in which a learner has to infer a deterministic finite automaton (DFA) for an unknown regular language L by asking queries to a teacher. The learner may pose two types of queries: "Is the word w in L?" (*membership queries*), and "Is the language recognized by DFA H equal to L?" (*equivalence queries*). In case of a *no* answer to an equivalence query, the teacher supplies a counterexample that distinguishes hypothesis H from L. The L^* algorithm proposed by Angluin [5] is able to learn L by asking a polynomial number of membership and equivalence queries (polynomial in the size of the corresponding canonical DFA).

Angluin's approach triggered a lot of subsequent research on active automata learning and has numerous applications in the area of software and hardware

* Research supported by NWO TOP project 612.001.852 "Grey-box learning of Interfaces for Refactoring Legacy Software (GIRLS)".

D. Fisman and G. Rosu (Eds.): TACAS 2022, LNCS 13243, pp. 223–243, 2022.
https://doi.org/10.1007/978-3-030-99524-9_12

analysis, for instance for generating conformance test suites of software components [28], finding bugs in implementations of security-critical protocols [22,23,21], learning interfaces of classes in software libraries [33], inferring interface protocols of legacy software components [8], and checking that a legacy component and a refactored implementation have the same behavior [55]. We refer to [63,34] for surveys and further references.

Since 1987, major improvements of the original L^* algorithm have been proposed, for instance by [52,53,38,41,56,35,45,50,32,37,25]. Yet, all these improvements are variations of L^* in the sense that they approximate the Nerode congruence by means of refinement. Isberner [36] shows that these *descendants* of L^* can be described in a single, general framework.[1]

Variations of L^* have also been used as a basis for learning extensions of DFAs such as Mealy machines [48], I/O automata [2], non-deterministic automata [16], alternating automata [6], register automata [1,17], nominal automata [46], symbolic automata [40,7], weighted automata [14,11,30], Mealy machines with timers [64], visibly pushdown automata [36], and categorical generalisations of automata [62,29,12,18]. It is fair to say that L^*-like algorithms completely dominate the research area of active automata learning.

In this paper we present $L^\#$, a fresh approach to automata learning that differs from L^* and its descendants. Instead of focusing on equivalence of observations, $L^\#$ tries to establish *apartness*, a constructive form of inequality [61,26]. The notion of apartness is standard in constructive real analysis and goes back to Brouwer, with Heyting giving an axiomatic treatment in [31]. This change in perspective has several key consequences, developed and presented in this paper:

- $L^\#$ does not maintain auxiliary data structures such as observation tables or discrimination trees, but operates directly on the observation tree. This tree is a partial Mealy machine itself, and is very close to an actual hypothesis that can be submitted to the teacher. As a result, our algorithm is *simple*.
- The asymptotic query complexity of $L^\#$ is $\mathcal{O}(kn^2 + n \log m)$ and the asymptotic symbol complexity[2] is $\mathcal{O}(kmn^2 + nm \log m)$. Here k is the number of input symbols, n is the number of states, and m is the length of the longest counterexample. These are the *same asymptotic complexities* as the best existing (L^*-like) learning algorithms [52,53,32,37,36,25].
- The use of observation trees as primary data structure makes it easy to *integrate concepts from conformance testing to improve the performance* of $L^\#$. In particular, adaptive distinguishing sequences [39], which we can compute directly from the observation tree, turn out to be an effective boost in practice, even if their use does not affect asymptotic complexities. Through $L^\#$ testing and learning become even more intertwined [13,4].

[1] Except for the ZQ algorithm of [50], which was developed independently, and the ADT algorithm of [25], that was developed later and uses adaptive distinguishing sequences which are not covered in Isberner's framework.

[2] The symbol complexity is the number of input symbols required to learn an automaton. This is a relevant measure for practical learning scenarios, where the total time needed to learn a model is proportional to the number of input symbols.

– Experiments on benchmarks of [47], with a *prototype implementation* written in Rust, suggest that $L^\#$ is competitive with existing, highly optimized algorithms implemented in LearnLib [51].

Related work. Despite the different data structures, $L^\#$ and L^* [5] still have many similarities, since both store all the information gained from all queries so far. Moreover, both maintain a set of those states that have been learned with absolute certainty already. A few other algorithms have been proposed that follow a different approach than L^*. Meinke [43,44] developed a dual approach where, instead of starting with a maximally coarse approximating relation and refining it during learning, one starts with a maximally fine relation and coarsens it by merging equivalence classes. Although Meinke reports superior performance in the application to learning-based testing, these algorithms have exponential worst-case query complexities. Using ideas from [53], Groz et al. [27] use a combination of homing sequences and characterization sets to develop an algorithm for active model learning that does not require the ability to reset the system. Via an extensive experimental evaluation involving benchmarks from [47] they show that the performance of their algorithm is competitive with the L^* descendant of [56], but there can be huge differences in the performance of their algorithm for models that are similar in size and structure. Several authors have explored the use of SAT and SMT solvers for obtaining learning algorithms, see for instance [49,58], but these approaches suffer from fundamental scalability problems. In a recent paper, Soucha & Bogdanov [60] outline an active learning algorithm which also takes the observation tree as the primary data structure, and use results from conformance testing to speed up learning. They report that an implementation of their approach outperforms standard learning algorithms like L^*, but they have no explicit apartness relation and associated theoretical framework. It is precisely this theoretical underpinning which allowed us to establish complexity and correctness results, and define efficient procedures for counterexample processing and computing adaptive distinguishing sequences.

In the present paper, we first define partial Mealy machines, observation trees, and apartness (Section 2). Then, we present the full $L^\#$ algorithm (Section 3) and benchmark our prototype implementation (Section 4). The proofs of all theorems and complete benchmark results can be found in the appendix of the full version [65] of this paper.

2 Partial Mealy Machines and Apartness

The $L^\#$ algorithm learns a hidden (complete) Mealy machine, and its primary data structure is a *partial* Mealy machine. We first fix notation for partial maps.

We write $f\colon X \rightharpoonup Y$ to denote that f is a partial function from X to Y and write $f(x)\!\downarrow$ to mean that f is defined on x, that is, $\exists y \in Y\colon f(x) = y$, and conversely write $f(x)\!\uparrow$ if f is undefined for x. Often, we identify a partial function $f\colon X \rightharpoonup Y$ with the set $\{(x, y) \in X \times Y \mid f(x) = y\}$. The composition of partial maps $f\colon X \rightharpoonup Y$ and $g\colon Y \rightharpoonup Z$ is denoted by $g \circ f\colon X \rightharpoonup Z$, and we have

$(g \circ f)(x)\!\downarrow$ iff $f(x)\!\downarrow$ and $g(f(x))\!\downarrow$. There is a partial order on $X \rightharpoonup Y$ defined by $f \sqsubseteq g$ for $f, g\colon X \rightharpoonup Y$ if for all $x \in X$, $f(x)\!\downarrow$ implies $g(x)\!\downarrow$ and $f(x) = g(x)$.

Throughout this paper, we fix a finite set I of *inputs* and a set O of *outputs*.

Definition 2.1. *A **Mealy machine** is a tuple $\mathcal{M} = (Q, q_0, \delta, \lambda)$, where*

- *Q is a finite set of **states** and $q_0 \in Q$ is the **initial state**,*
- *$\langle \lambda, \delta \rangle\colon Q \times I \rightharpoonup O \times Q$ is a partial map whose components are an **output function** $\lambda\colon Q \times I \rightharpoonup O$ and a **transition function** $\delta\colon Q \times I \rightharpoonup Q$ (hence, $\delta(q,i)\!\downarrow \Leftrightarrow \lambda(q,i)\!\downarrow$, for $q \in Q$ and $i \in I$).*

*We use superscript $\mathcal{M}$ to disambiguate to which Mealy machine we refer, e.g. $Q^{\mathcal{M}}$, $q_0^{\mathcal{M}}$, $\delta^{\mathcal{M}}$ and $\lambda^{\mathcal{M}}$. We write $q \xrightarrow{i/o} q'$, for $q, q' \in Q$, $i \in I$, $o \in O$ to denote $\lambda(q,i) = o$ and $\delta(q,i) = q'$. We call $\mathcal{M}$ **complete** if δ is total, i.e., $\delta(q,i)$ is defined for all states q and inputs i. We generalize the transition and output functions to input words of length $n \in \mathbb{N}$ by composing $\langle \lambda, \delta \rangle$ n times with itself: we define maps $\langle \lambda_n, \delta_n \rangle\colon Q \times I^n \to O^n \times Q$ by $\langle \lambda_0, \delta_0 \rangle = \mathsf{id}_Q$ and*

$$\langle \lambda_{n+1}, \delta_{n+1} \rangle\colon \; Q \times I^{n+1} \xrightarrow{\langle \lambda_n, \delta_n \rangle \times \mathsf{id}_I} O^n \times Q \times I \xrightarrow{\mathsf{id}_{O^n} \times \langle \lambda, \delta \rangle} O^{n+1} \times Q$$

Whenever it is clear from the context, we use λ and δ also for words.

Definition 2.2. *The semantics of a state q is a map $[\![q]\!]\colon I^* \rightharpoonup O^*$ defined by $[\![q]\!](\sigma) = \lambda(q, \sigma)$. States q, q' in possibly different Mealy machines are **equivalent**, written $q \approx q'$, if $[\![q]\!] = [\![q']\!]$. Mealy machines $\mathcal{M}$ and $\mathcal{N}$ are **equivalent** if their respective initial states are equivalent: $q_0^{\mathcal{M}} \approx q_0^{\mathcal{N}}$.*

In our learning setting, an *undefined* value in the partial transition map represents lack of knowledge. We consider maps between Mealy machines that preserve existing transitions, but possibly extend the knowledge of transitions:

Definition 2.3. *For Mealy machines $\mathcal{M}$ and $\mathcal{N}$, a **functional simulation** $f\colon \mathcal{M} \to \mathcal{N}$ is a map $f\colon Q^{\mathcal{M}} \to Q^{\mathcal{N}}$ with*

$$f(q_0^{\mathcal{M}}) = q_0^{\mathcal{N}} \qquad \text{and} \qquad q \xrightarrow{i/o} q' \text{ implies } f(q) \xrightarrow{i/o} f(q').$$

Intuitively, a functional simulation preserves transitions. In the literature, a functional simulation is also called *refinement mapping* [3].

Lemma 2.4. *For a functional simulation $f\colon \mathcal{M} \to \mathcal{N}$ and $q \in Q^{\mathcal{M}}$, we have $[\![q]\!] \sqsubseteq [\![f(q)]\!]$.*

For a given machine $\mathcal{M}$, an observation tree is simply a Mealy machine itself which represents the inputs and outputs we have observed so far during learning. Using functional simulations, we define it formally as follows.

Definition 2.5 ((Observation) Tree). *A Mealy machine $\mathcal{T}$ is a **tree** if for each $q \in Q^{\mathcal{T}}$ there is a unique sequence $\sigma \in I^*$ s.t. $\delta^{\mathcal{T}}(q_0^{\mathcal{T}}, \sigma) = q$. We write $\mathsf{access}(q)$ for the sequence of inputs leading to q. A tree $\mathcal{T}$ is an **observation tree** for a Mealy machine $\mathcal{M}$ if there is a functional simulation $f\colon \mathcal{T} \to \mathcal{M}$.*

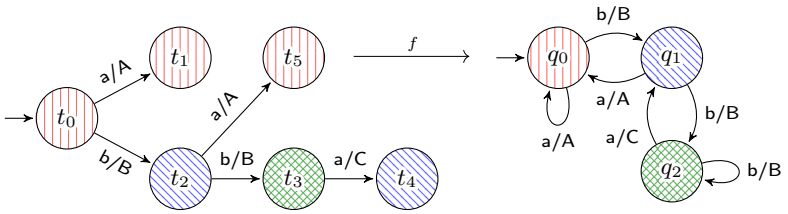


Fig. 1: An observation tree (left) for a Mealy machine (right).

Figure 1 shows an observation tree for the Mealy machine displayed on the right. The functional simulation f is indicated via coloring of the states.

By performing output and equivalence queries, the learner can build an observation tree for the unknown Mealy machine $\mathcal{M}$ of the teacher. However, the learner does not know the functional simulation. Nevertheless, by analysis of the observation tree, the learner may infer that certain states in the tree cannot have the same color, that is, they cannot be mapped to same states of $\mathcal{M}$ by a functional simulation. In this analysis, the concept of *apartness*, a constructive form of inequality, plays a crucial role [61,26]. A similar concept has previously been studied in the context of automata learning under the name *inequivalence constraints* in work on passive learning of DFAs, see for instance [15,24].

Definition 2.6. *For a Mealy machine $\mathcal{M}$, we say that states $q, p \in Q^{\mathcal{M}}$ are **apart** (written $q \# p$) if there is some $\sigma \in I^*$ such that $[\![q]\!](\sigma)\!\downarrow$, $[\![p]\!](\sigma)\!\downarrow$, and $[\![q]\!](\sigma) \neq [\![p]\!](\sigma)$. We say that σ is the **witness** of $q \# p$ and write $\sigma \vdash q \# p$.*

Note that the apartness relation $\# \subseteq Q \times Q$ is irreflexive and symmetric. A witness is also called *separating sequence* [59]. For the observation tree of Figure 1 we may derive the following apartness pairs and corresponding witnesses:

$$a \vdash t_0 \# t_3 \qquad a \vdash t_2 \# t_3 \qquad b\,a \vdash t_0 \# t_2$$

The apartness of states $q \# p$ expresses that there is a conflict in their semantics, and consequently, apart states can never be identified by a functional simulation:

Lemma 2.7. *For a functional simulation $f \colon \mathcal{T} \to \mathcal{M}$,*

$$q \# p \text{ in } \mathcal{T} \qquad \Longrightarrow \qquad f(q) \not\approx f(p) \text{ in } \mathcal{M} \qquad \text{for all } q, p \in Q^{\mathcal{T}}.$$

Thus, whenever states are apart in the observation tree $\mathcal{T}$, the learner knows that these are distinct states in the hidden Mealy machine $\mathcal{M}$.

The apartness relation satisfies a weaker version of *co-transitivity*, stating that if $\sigma \vdash r \# r'$ and q has the transitions for σ, then q must be apart from at least one of r and r', or maybe even both:

Lemma 2.8 (Weak co-transitivity). *In every Mealy machine $\mathcal{M}$,*

$$\sigma \vdash r \# r' \ \wedge \ \delta(q, \sigma)\!\downarrow \ \Longrightarrow \ r \# q \ \vee \ r' \# q \qquad \text{for all } r, r', q \in Q^{\mathcal{M}}, \sigma \in I^*.$$

We use the weak co-transitivity property during learning. For instance in Fig. 1, by posing the output query *aba*, consisting of the access sequence for t_1 concatenated with the witness *ba* for $t_0 \# t_2$, co-transitivity ensures that $t_0 \# t_1$ or $t_2 \# t_1$. By inspecting the outputs, the learner may conclude that $t_2 \# t_1$.

3 Learning Algorithm

The task solved by $L^\#$ is to find a strategy for the learner in the following game:

Definition 3.1. *In the learning game between a learner and a teacher, the teacher has a complete Mealy machine $\mathcal{M}$ and answers the following queries from the learner:*

OutputQuery(σ)**:** *For $\sigma \in I^*$, the teacher replies with the corresponding output sequence $\lambda^{\mathcal{M}}(q_0^{\mathcal{M}}, \sigma) \in O^*$.*[3]

EquivQuery$(\mathcal{H})$**:** *For a complete Mealy machine $\mathcal{H}$, the teacher replies* `yes` *if $\mathcal{H} \approx \mathcal{M}$ or* `no`*, providing some $\sigma \in I^*$ with $\lambda^{\mathcal{M}}(q_0^{\mathcal{M}}, \sigma) \neq \lambda^{\mathcal{H}}(q_0^{\mathcal{H}}, \sigma)$.*

Our $L^\#$ algorithm operates on an observation tree $\mathcal{T} = (Q, q_0, \delta, \lambda)$ for the unknown complete Mealy machine $\mathcal{M}$, where $\mathcal{T}$ contains the results of all output and equivalence queries so far. An observation tree is similar to the *cache* which is commonly used in implementations of L^*-based learning algorithms to store the answers to previously asked queries, avoiding duplicates [10,42]. But whereas for L^*-based learning algorithms the cache is an auxiliary data structure and only used for efficiency reasons, it is a first-class citizen in $L^\#$.

Remark 3.2. The learner has no information about the teacher's hidden Mealy machine. In particular, whenever we write #, we always refer to the apartness relation *on the observation tree* $\mathcal{T}$.

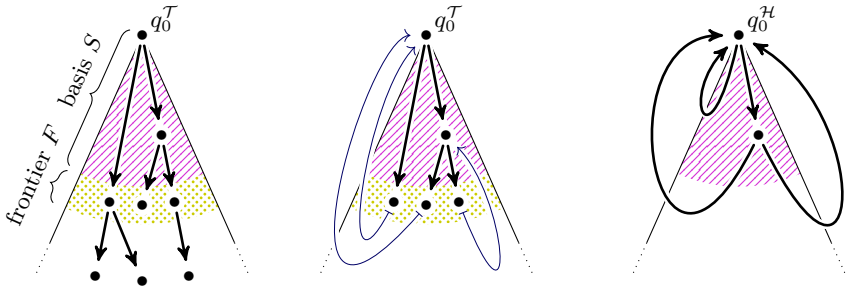
The observation tree is structured in a very similar way as Dijkstra's shortest path algorithm [19] structures a graph. Recall that during the execution of Dijkstra's algorithm 'the nodes are subdivided into three sets' [19]:

1. the nodes S to which a shortest path from the initial node is known. S initially only contains the initial node and grows from there.
2. the nodes F from which the next node to be added to S will be selected.
3. the remaining nodes.

This scheme adapts to the observation tree as follows and is visualized in Fig. 2a.

1. The states $S \subseteq Q^{\mathcal{T}}$, which already have been fully identified, i.e. the learner found out that these must represent distinct states in the teacher's hidden Mealy machine. We call S the *basis*. Initially, $S := \{q_0^{\mathcal{T}}\}$, and throughout the execution S forms a subtree of $\mathcal{T}$ and all states in S are pairwise apart: $\forall p, q \in S, p \neq q \colon p \# q$.

[3] In fact, later on we will assume that the teacher responds to slightly more general output queries to enable the use of *adaptive distinguishing sequences*, see Section 3.5.



(a) $\mathcal{T}$, S, and F (b) A choice $h\colon F \to S$ (c) Hypothesis $\mathcal{H}$ for h

Fig. 2: From the observation tree to the hypothesis ($|I| = 2$)

2. the *frontier* $F \subseteq Q^{\mathcal{T}}$, from which the next node to be added to S is chosen. Throughout the execution, F is the set of immediate non-basis successors of basis states: $F := \{q' \in Q \setminus S \mid \exists q \in S, i \in I : q' = \delta(q, i)\}$.
3. the remaining states $Q \setminus (S \cup F)$.

Initially, $\mathcal{T}$ consists of only an initial state $q_0^{\mathcal{T}}$ with no transitions. For every OutputQuery(σ) during the execution, the input $\sigma \in I^*$ and the corresponding response of type O^* is added automatically to the observation tree $\mathcal{T}$, and similarly every negative response to a EquivQuery leads to new states and transitions in the observation tree. With every extension $\mathcal{T}'$ of the observation tree $\mathcal{T}$, the apartness relation can only grow: whenever $p \# q$ in $\mathcal{T}$, then still $p \# q$ in $\mathcal{T}'$. Thus, along the learning game, $\mathcal{T}$ and $\#$ grow steadily:

Assumption 3.3 *We implicitly require that via output and equivalence queries, the observation tree $\mathcal{T}$ and the basis S are gradually extended, with the frontier F automatically moving along while S grows.*

3.1 Hypothesis construction

At almost any point during the learning game, the learner can come up with a hypothesis $\mathcal{H}$ based on the knowledge in the observation tree $\mathcal{T}$. Since the basis S contains the states already discovered, the set of states of such a hypothesis is simply set to $Q^{\mathcal{H}} := S$, and it contains every transition between basis states (in $\mathcal{T}$). The hypothesis must also reflect the transitions in $\mathcal{T}$ that leave the basis S, i.e. the transitions to the frontier. Those are resolved by finding for every frontier state a base state, for which the learner conjectures that they are equivalent states in the hidden Mealy machine. This choice boils down to a map $h\colon F \to S$ ($\mapsto$ in Fig. 2b). Then, a transition $q \xrightarrow{i/o} p$ in $\mathcal{T}$ with $q \in S$, $p \in F$ leads to a transition $q \xrightarrow{i/o} h(p)$ in $\mathcal{H}$ (Fig. 2c). These ideas are formally defined as follows.

Definition 3.4. *Let $\mathcal{T}$ be an observation tree with basis S and frontier F.*

1. *A Mealy machine $\mathcal{H}$ **contains the basis** if $Q^{\mathcal{H}} = S$ and $\delta^{\mathcal{H}}(q_0^{\mathcal{H}}, \mathsf{access}(q)) = q$ for all $q \in S$.*

2. *A* ***hypothesis*** *is a complete Mealy machine $\mathcal{H}$ containing the basis such that $q \xrightarrow{i/o'} p'$ in $\mathcal{H}$ $(q \in S)$ and $q \xrightarrow{i/o} p$ in $\mathcal{T}$ imply $o = o'$ and $\neg(p \# p')$ (in $\mathcal{T}$).*
3. *A hypothesis $\mathcal{H}$ is* ***consistent*** *if there is a functional simulation $f : \mathcal{T} \to \mathcal{H}$.*
4. *For a Mealy machine $\mathcal{H}$ containing the basis, an input sequence $\sigma \in I^*$ is said to* ***lead to a conflict*** *if $\delta^{\mathcal{T}}(q_0^{\mathcal{T}}, \sigma) \# \delta^{\mathcal{H}}(q_0^{\mathcal{H}}, \sigma)$ (in $\mathcal{T}$).*

Intuitively, the first three notions describe how confident we are in the correctness of the 'back loops' in $\mathcal{H}$ obtained from a choice $h : F \to S$. Notion 1 does not provide any warranty, notion 2 asserts that $\neg(q \# h(q))$ for all $q \in F$, and notion 3 (by definition) means that $\mathcal{T}$ is an observation tree for $\mathcal{H}$, that is, all observations so far are consistent with the hypothesis $\mathcal{H}$. The learner can verify the consistency of a hypothesis without querying the teacher (algorithm is in Section 3.3 below). The existence and uniqueness of a hypothesis are related to criteria on $\mathcal{T}$:

Definition 3.5. *In an observation tree $\mathcal{T}$, a state in F is 1.* ***isolated*** *if it is apart from all states in S and 2. is* ***identified*** *if it is apart from all states in S except one. 3. The basis S is* ***complete*** *if each state in S has a transition for each input in I.*

Lemma 3.6. *For an observation tree $\mathcal{T}$, if F has no isolated states then there exists a hypothesis $\mathcal{H}$ for $\mathcal{T}$. If S is complete and all states in F are identified then the hypothesis is unique.*

With a growing observation tree $\mathcal{T}$, the hidden Mealy machine is found as soon as the basis is big enough:

Theorem 3.7. *Suppose $\mathcal{T}$ is an observation tree for a (hidden) Mealy machine $\mathcal{M}$ such that S is complete, all states in F are identified, and $|S|$ is the number of equivalence classes of $\approx^{\mathcal{M}}$. Then $\mathcal{H} \approx \mathcal{M}$ for the unique hypothesis $\mathcal{H}$.*

The theorem itself is not necessary for the correctness of $L^{\#}$, but guarantees feasibility of learning.

3.2 Main loop of the algorithm

The $L^{\#}$ algorithm is listed in Algorithm 1 in pseudocode. The code uses Dijkstra's guarded command notation [20], which means that the following rules are applied non-deterministically until none of them can be applied anymore:

(R1) If F contains an isolated state, then this means that we have discovered a new state not yet present in S, hence we move it from F to S.

(R2) When a state $q \in S$ has no outgoing i-transition, for some $i \in I$, the output query for $\mathsf{access}(q)\ i$ will add the generated i successor, implicitly extending the frontier F.

Algorithm 1 Overall $L^\#$ algorithm

```
procedure LSharp
    do q isolated, for some q ∈ F →                                   ▷ Rule (R1)
        S ← S ∪ {q}
    □ δ^T(q, i) ↑, for some q ∈ S, i ∈ I →                             ▷ Rule (R2)
        OutputQuery(access(q) i)
    □ ¬(q # r), ¬(q # r'), for some q ∈ F, r, r' ∈ S, r ≠ r' →         ▷ Rule (R3)
        σ ← witness of r # r'
        OutputQuery(access(q) σ)
    □ F has no isolated states and basis S is complete →              ▷ Rule (R4)
        H ← BuildHypothesis
        (b, σ) ← CheckConsistency(H)
        if b = yes then
            (b, ρ) ← EquivQuery(H)
            if b = yes then: return H
            else: σ ← shortest prefix of ρ such that δ^H(q_0^H, σ) # δ^T(q_0^T, σ) (in T)
        end if
        ProcCounterEx(H, σ)
    end do
end procedure
```

(R3) When $q \in F$ is a state in the frontier that is not yet identified, then there are at least two states in S that are not apart from q. In this case, the algorithm picks a witness $\sigma \in I^*$ for $r \# r'$. After the OutputQuery(access$(q)\,\sigma$), the observation tree is extended and thus q will be apart from at least r or r' by weak co-transitivity (Lemma 2.8).

(R4) When F has no isolated states and S is complete, BuildHypothesis picks a hypothesis $\mathcal{H}$ (at least one exists Lemma 3.6). If $\mathcal{H}$ is not consistent with observation tree $\mathcal{T}$ we get a conflict σ for free. Otherwise, we pose an equivalence query for $\mathcal{H}$. If the hypothesis is correct, $L^\#$ terminates, and otherwise we obtain a counterexample ρ. The counterexample decomposes into two words $\sigma\eta$, where σ leads to a conflict and η witnesses it. The conflict σ means that one of the frontier states was merged with an apart basis state in $\mathcal{H}$, causing a wrong transition in $\mathcal{H}$. Since σ can be very long, the task of ProcCounterEx(σ) is to shorten σ until we know which frontier state caused the conflict. So after ProcCounterEx, $\mathcal{H}$ is not a hypothesis for the updated $\mathcal{T}$ anymore.

We will show the correctness of $L^\#$ in a top-down approach discussing the subroutines later and only assuming now that:

1. BuildHypothesis picks one of the possible hypotheses (Lemma 3.6)
2. CheckConsistency$(\mathcal{H})$ tells if there is a functional simulation $\mathcal{T} \to \mathcal{H}$, and if not, provides $\sigma \in I^*$ leading to a conflict (Lemma 3.10 below).
3. If $\mathcal{H}$ contains the basis and σ leads to a conflict, then ProcCounterEx$(\mathcal{H}, \sigma)$, extends $\mathcal{T}$ such that $\mathcal{H}$ is not a hypothesis anymore (Lemma 3.11 below).

Whenever the algorithm terminates, the learner has found the correct model. Therefore, correctness amounts to showing termination. The rough idea is that each rule will let S, F, or $\#$ restricted to $S \times F$ grow, and each of these sets are bounded by the hidden Mealy machine $\mathcal{M}$. We define the norm $N(\mathcal{T})$ by

$$\frac{|S| \cdot (|S|+1)}{2} \;+\; |\{(q,i) \in S \times I \mid \delta^{\mathcal{T}}(q,i)\!\downarrow\}| \;+\; |\{(q,q') \in S \times F \mid q \# q'\}| \quad (1)$$

The first summand increases whenever a state is moved from F to S (R1); it is quadratic in $|S|$ because (R1) reduces the third summand. The second summand records the progress achieved by extending the frontier (R2). The third summand counts how much the states in the frontier are identified (R3). Rule (R4) extends the apartness relation, leading to an increase of the third summand.

Theorem 3.8. *Every rule application in $L^{\#}$ increases the norm $N(\mathcal{T})$ in (1).*

The norm $N(\mathcal{T})$ and therefore also the number of rule applications is bounded:

Theorem 3.9. *If $\mathcal{T}$ is an observation tree for $\mathcal{M}$ with n equivalence classes of states and $|I| = k$, then $N(\mathcal{T}) \leq \frac{1}{2} \cdot n \cdot (n+1) + kn + (n-1)(kn+1) \in \mathcal{O}(kn^2)$.*

At any point of execution, either rule (R1), (R2), or (R4) is applicable, so $L^{\#}$ never blocks. As soon as the norm $N(\mathcal{T})$ hits the bound, the only applicable rule is rule (R4) with the teacher accepting the hypothesis. Thus, the correct Mealy machine is learned within $\mathcal{O}(k \cdot n^2)$ rule applications. The complexity in terms of the input parameters is studied in Section 3.6.

We now continue defining the subroutines and proving them correct.

3.3 Consistency checking

A hypothesis $\mathcal{H}$ is not necessarily *consistent* with $\mathcal{T}$, in the sense of a functional simulation $\mathcal{T} \to \mathcal{H}$. Via a breadth-first search of the Cartesian product of $\mathcal{T}$ and $\mathcal{H}$ (Algorithm 2), we may check in time linear in the size of $\mathcal{T}$ whether a functional simulation $\mathcal{T} \to \mathcal{H}$ exists. In the negative case, we obtain $\sigma \in I^*$ leading to a conflict without any equivalence or output query to the teacher needed. Thus, this is also called 'counterexample milking' [10].

Lemma 3.10. *Algorithm 2 terminates and is correct, that is, if $\mathcal{H}$ is a hypothesis for $\mathcal{T}$ with a complete basis, then* CheckConsistency$(\mathcal{H})$

1. *returns* `yes`*, if $\mathcal{H}$ is consistent,*
2. *returns* `no` *and $\rho \in I^*$, if ρ leads to a conflict ($\delta^{\mathcal{T}}(q_0^{\mathcal{T}}, \rho) \# \delta^{\mathcal{H}}(q_0^{\mathcal{H}}, \rho)$ in $\mathcal{T}$).*

3.4 Counterexample processing

The L^* algorithm [5] performs $\mathcal{O}(m)$ queries to analyze a counterexample of length m. So if a teacher returns really long counterexamples, their analysis will dominate the learning process. Rivest & Schapire [52,53] improve counterexample

Algorithm 2 Check if hypothesis $\mathcal{H}$ is consistent with observation tree $\mathcal{T}$

```
procedure CheckConsistency(H)
    Q ← new queue ⊆ S × S
    enqueue(Q, (q_0^T, q_0^H)))
    while (q, r) ← dequeue(Q)
        if q # r then: return no: access(q)
        for all q --i/o--> p in T do
            enqueue(Q, (p, δ^H(r, i)))
        end for
    end while
    return yes
end procedure
```

analysis of L^* using binary search, requiring only $\mathcal{O}(\log m)$ queries. A similar trick is applied in $L^\#$.

Suppose σ leads to a conflict $q \# r$ for $q = \delta^{\mathcal{H}}(q_0^{\mathcal{H}}, \sigma)$ and $r = \delta^{\mathcal{T}}(q_0^{\mathcal{T}}, \sigma)$. Then, ProcCounterEx($\sigma$) (Algorithm 3) extends $\mathcal{T}$ such that $\mathcal{H}$ will never be a hypothesis for $\mathcal{T}$ again.

If $r \in S \cup F$, then the conflict $q \# r$ is obvious and $\mathcal{H}$ is not a hypothesis again. If otherwise $r \notin S \cup F$, the binary search will successively reduce the number of transitions of σ outside $S \cup F$ by a factor of 2 until we reach the above base case $S \cup F$. Let $\sigma_1 \sigma_2 := \sigma$ such that the run of σ_1 in $\mathcal{T}$ ends halfway between the frontier and r. By an additional output query, the binary search checks whether already σ_1 leads to a conflict. In the two cases, we can either avoid σ_1 or σ_2, so we reduce the number of transitions outside $S \cup F$ to half the amount. The precise argument is in:

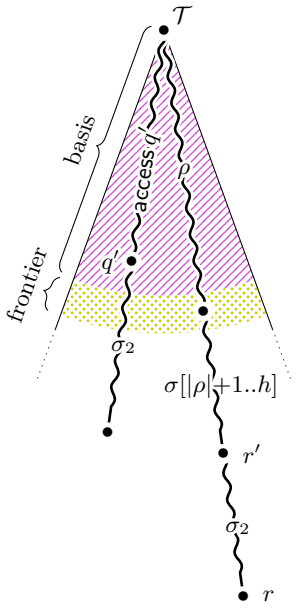
Lemma 3.11. *Suppose basis S is complete, $\mathcal{H}$ is a complete Mealy machine containing the basis, and $\sigma \in I^*$ leads to a conflict. Then* ProcCounterEx($\mathcal{H}, \sigma$) *terminates, performs at most $\mathcal{O}(\log_2 |\sigma|)$ output queries and is correct: upon termination, the machine $\mathcal{H}$ is not a hypothesis for $\mathcal{T}$ anymore.*

3.5 Adaptive distinguishing sequences

As an optimization in practice, we may extend the rules (R2) and (R3) by incorporating *adaptive distinguishing sequences* (Ads) into the respective output queries. Adaptive distinguishing sequences, which are commonly used in the area of conformance testing [39], are input sequences where the choice of an input may depend on the outputs received in response to previous inputs. Thus, strictly speaking, an ADS is a decision graph rather than a sequence. This mild extension of the learning framework reflects the actual black box behaviour of Mealy machines: for every input in I sent to the hidden Mealy machine, the learner observes the output O before sending the next input symbol. Use of adaptive distinguishing sequences may reduce the number of output queries that are required for the identification of frontier states.

Algorithm 3 Processing σ that leads to a conflict, i.e. $\delta^{\mathcal{H}}(q_0, \sigma) \# \delta^{\mathcal{T}}(q_0, \sigma)$

procedure ProcCounterEx($\mathcal{H}$, $\sigma \in I^*$)
  $q \leftarrow \delta^{\mathcal{H}}(q_0^{\mathcal{H}}, \sigma)$
  $r \leftarrow \delta^{\mathcal{T}}(q_0^{\mathcal{T}}, \sigma)$
  if $r \in S \cup F$ **then**
    return
  else
    $\rho \leftarrow$ unique prefix of σ with $\delta^{\mathcal{T}}(q_0^{\mathcal{T}}, \rho) \in F$
    $h \leftarrow \lfloor \frac{|\rho|+|\sigma|}{2} \rfloor$
    $\sigma_1 \leftarrow \sigma[1..h]$
    $\sigma_2 \leftarrow \sigma[h+1..|\sigma|]$
    $q' \leftarrow \delta^{\mathcal{H}}(q_0^{\mathcal{H}}, \sigma_1)$
    $r' \leftarrow \delta^{\mathcal{T}}(q_0^{\mathcal{T}}, \sigma_1)$
    $\eta \leftarrow$ witness for $q \# r$
    OutputQuery(access(q') σ_2 η)
    if $q' \# r'$ **then**
      ProcCounterEx ($\mathcal{H}$, σ_1)
    else
      ProcCounterEx ($\mathcal{H}$, access(q') σ_2)
    end if
  end if
end procedure



As an example, consider the observation tree of Figure 3(left). The basis for this tree consists of 5 states, which are pairwise apart (separating sequences are a, ab and aa). Frontier states can be identified by the *single* adaptive sequence of Figure 3(right). The ADS starts with input a. If the response is 2 we have identified our frontier state as t_4. If the response is 0 then the frontier state is either t_0 or t_2, and we may identify the state with a subsequent input a. Similarly, if the response is 1 then the frontier state is either t_1 or t_3, and we may identify the state by a subsequent input b. We can therefore identify (or isolate) frontier state t_5 with a single (extended) output query that starts with the access sequence for t_5 ($bbbba$) followed by the ADS of Figure 3(right). If we used separating sequences, we would need at least 2 output queries.

In the setting of $L^{\#}$, we can directly compute an optimal ADS from the current observation tree. To this end, we recursively define an *expected reward* function E, which sends a set $U \subseteq Q^{\mathcal{T}}$ of states to the maximal expected number of apartness pairs (in the absence of unexpected outputs).

$$E(U) = \max_{i \in inp(U)} \left(\sum_{o \in O} \frac{|U \xrightarrow{i/o}| \cdot (|U \xrightarrow{i}| - |U \xrightarrow{i/o}| + E(U \xrightarrow{i/o}))}{|U \xrightarrow{i}|} \right) \tag{2}$$

where $inp(U) := \{i \in I \mid \exists q \in U : \delta^{\mathcal{T}}(q, i)\!\downarrow\}$, $U \xrightarrow{i} := \{q \in U \mid \delta^{\mathcal{T}}(q, i)\!\downarrow\}$ and $U \xrightarrow{i/o} := \{q' \in Q^{\mathcal{T}} \mid \exists q \in U : q \xrightarrow{i/o} q'\}$. We define the maximum over the empty set to be 0. Then Ads(U) is the decision tree constructed as follows:

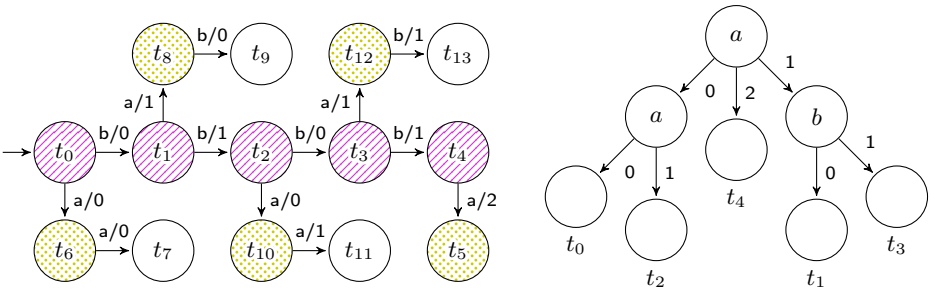


Fig. 3: An observation tree (left) and an ADS for its basis (right)

- If $U \xrightarrow{i} = \emptyset$ then $\textsc{Ads}(U)$ consists of a single node U without a label.
- If $U \xrightarrow{i} \neq \emptyset$ then $\textsc{Ads}(U)$ is constructed by choosing an input i that witnesses the maximum $E(U)$, creating a node U with label i, and, for each output o with $U \xrightarrow{i/o} \neq \emptyset$, adding an o-transition to $ADS(U \xrightarrow{i/o})$.

For the observation tree of Figure 3(left) we may compute $E(\{t_0, \ldots, t_4\}) = 4$ and obtain the decision tree of Figure 3(right) as ADS. Running the ADS from state t_5 will create 4 new apartness pairs with basis states (or 5 in case an unexpected output occurs, e.g. $a(1)b(2)$).

Proposition 3.12. *Define $L^{\#}_{\textsc{Ads}}$ by replacing the output queries in $L^{\#}$ with*

(R2') $\textsc{OutputQuery}(\mathsf{access}(q)\ i\ \textsc{Ads}(S))$ *in (R2) and*
(R3') $\textsc{OutputQuery}(\mathsf{access}(q)\ \textsc{Ads}(\{b \in S \mid \neg(b \# q)\}))$ *in (R3).*

Then, $L^{\#}_{\textsc{Ads}}$ lets the norm $N(\mathcal{T})$ grow for each rule application and thus is correct.

3.6 Complexity

Since equivalence queries are costly in practice and since processing of long counterexamples of length m requires $\mathcal{O}(\log m)$ output queries, it makes sense to postpone equivalence queries as long as possible:

Definition 3.13. ***Strategic*** *$L^{\#}$ (resp. $L^{\#}_{\textsc{Ads}}$) is the special case of Algorithm 1 where rule (R4) is only applied if none of the other rules is applicable.*

Then we obtain the following query complexity for the $L^{\#}$ algorithm.

Theorem 3.14. *Strategic $L^{\#}$ (resp. $L^{\#}_{\textsc{Ads}}$) learns the correct Mealy machine within $\mathcal{O}(kn^2 + n \log m)$ output queries and at most $n - 1$ equivalence queries.*

The query complexity of $L^{\#}$ equals the best known query complexity for active learning algorithms, as achieved by Rivest & Schapire's algorithm [52,53], the observation pack algorithm [32], the TTT algorithm [37,36], and the ADT algorithm [25].

In a black box learning setting in practice, answering an output query for $\sigma \in I^*$ grows linearly with the length σ. Therefore, the (asymptotic) total number of input symbols sent by the learner is also a metric for comparing learning algorithms:

Theorem 3.15. *Let $n \in \mathcal{O}(m)$. Then the strategic $L^\#$ algorithm learns the correct Mealy machine with $\mathcal{O}(kmn^2 + nm \log m)$ input symbols.*

This matches the asymptotic symbol complexity of the best known active learning algorithms. Although ProcCounterEx reduces the length of the sequence leading to the conflict, the witness of the conflict remains of size $\Theta(m)$ in the worst case. This means that we need $\mathcal{O}(m \log m)$ symbols to process a single counterexample and $\mathcal{O}(nm \log m)$ symbols to process all counterexamples.

4 Experimental Evaluation

In the previous sections, we have introduced and discussed the $L^\#$ algorithm. We now present a short experimental evaluation of the algorithm to demonstrate its performance when compared to other state-of-art algorithms. We run two versions of $L^\#$: the base version (Algorithm 1), and the ADS optimised variant ($L^\#_{\text{ADS}}$), and compare these with the (highly optimized) LearnLib[4] implementations of TTT, ADT,[5] and 'RS', by which we refer to L^* with Rivest-Schapire counterexample processing [52,53]. All source-code and data is available online.[6]

Implementing EquivQuery*:* We implement equivalence queries using conformance testing, which also makes output queries. We have fixed the testing tool to Hybrid-ADS[7] [57]. Hybrid-ADS has multiple configuration options, and we have set the state cover mode to "buggy", the number of extra states to check for to 10, the number of infix symbols to 10, and the mode of execution to "random", generating an infinite test-suite. Note that with these settings, the equivalence queries are not exact in general but approximated via random testing.

Data-set and metrics: We use a subset of the models available from the AutomataWiki (see [47]): we learn models for the SSH, TCP, and TLS protocols, alongside the BankCard models. The largest model in this subset has 66 states and 13 input symbols. We record the number of output queries and input symbols used during learning and testing, alongside the number of equivalence queries required to learn each model. An output query is a sequence $\sigma \in I^*$ of $|\sigma|$ input symbols and one *reset* symbol. A reset symbol returns the *system under test* (SUT) to its initial state. So *resets* denotes the number of output queries and *inputs* denotes the total number of symbols sent to the SUT. We believe that these metrics accurately portray the effort required to learn a model.

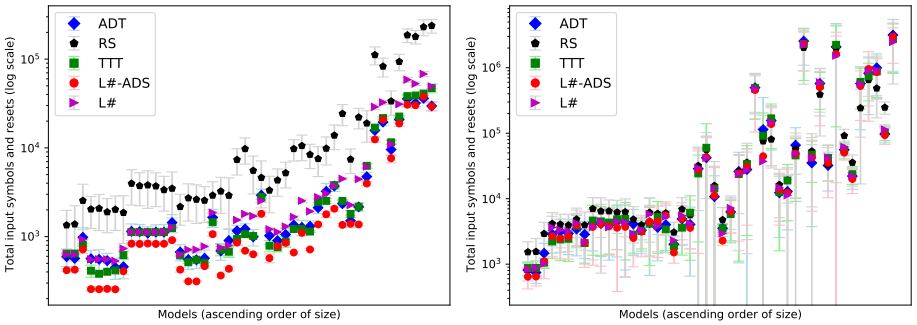
[4] https://learnlib.de/

[5] The ADT algorithm makes use of some heuristics to guide the learning process, we have selected the "Best-Effort" settings.

[6] https://gitlab.science.ru.nl/sws/lsharp and 10.5281/zenodo.5735533

[7] https://github.com/Jaxan/hybrid-ads

Experiment Set-up: All experiments were run on a Ryzen 3700X processor with 32GB of memory, running Linux. Each experiment refers to completely learning a model of the SUT. Due to the effects of randomization in the equivalence oracle, we repeat each experiment 100 times.



(a) Symbols used during learning phase (b) Symbols used both learning and testing

Fig. 4: Performance plots of the selected learning algorithms (lower is better.)

Results and Discussion Fig. 4a shows the total size of data sent by the learning algorithms via output queries – so both the number and the size of output queries are counted. In order to incorporate the equivalence queries, Fig. 4b shows the total size of data sent to the SUT during learning and testing. Note, in both plots the y-axis is log-scaled. The x-axis indicates the models, sorted in increasing number of states. The bars indicate standard deviation.

We can observe from the learning phase plot (Fig. 4a) that $L^{\#}$ expectedly does not perform better than the TTT and ADT algorithms, while the RS algorithm performs the worst among all four. However, $L^{\#}_{\text{ADS}}$ usually performs better than – or, at least, is competitive with – ADT and TTT. Furthermore, the error bars in the learning phase are very small, indicating that the measurements are stable. Generally, depending on the models a different algorithm is the fastest, but for every model, $L^{\#}_{\text{ADS}}$ is among the fastest, with and without the exclusion of the testing phase.

Fig. 4b presents the total number of input symbols and resets sent to the SUT. All algorithms seem to be very close in performance, which may be explained by the testing phase dominating the process. Indeed, Aslam et al. [8] experimentally demonstrated that it is largely the testing phase which influences learning effort.

The complete benchmark results (in the appendix of [65]) show more detailed information of the learned models, and highlights the smallest number per column and model. We can see that the number of equivalence queries are roughly similar for almost all the algorithms, while $L^{\#}$ seems to perform better for some models in the learning phase.

5 Conclusions and Future Work

We presented $L^\#$, a new algorithm for the classical problem of active automata learning. The key idea behind the approach is to focus on establishing *apartness*, or inequivalence of states, instead of approximating equivalence as in L^* and its descendants. Concretely, the table/discrimination tree in L^*-like algorithms is replaced in $L^\#$ by an observation tree, together with an apartness relation. This change in perspective leads to a simple but effective algorithm, which reduces the total number of symbols required for learning when compared to state-of-the-art algorithms. In particular, the use of observation trees, which are essentially tree-shaped Mealy machines, enables a modular integration of testing techniques, such as the ADS method, to identify states. Although the asymptotic output query complexity of $L^\#$ is $\mathcal{O}(kn^2 + n \log m)$, in our experiments $L^\#$ only needs in between kn and $4kn$ output queries (resets) to learn the benchmark models (with $n \leq 66$), which means that on average $L^\#$ needs in between 1 and 4 output queries to identify a frontier state.

Of course there are also similarities between $L^\#$ and L^*. The basis of $L^\#$ is comparable to the top half of the L^* table: both in $L^\#$ and in ([53]'s version of) L^* these prefixes induce a spanning tree. The frontier of $L^\#$ is comparable to the bottom half of the L^* table. But whereas L^* constructs residual classes of the language, $L^\#$ builds an automaton directly from the observation tree. As a consequence, L^* asks redundant queries, and optimizations of L^* try to avoid this redundancy. In contrast, $L^\#$ does not even think about asking redundant queries since it operates directly on the observation tree and only poses queries that increase the norm.

There is still much work to do to improve our prototype implementation, to include additional conformance testing algorithms, and to extend the experimental evaluation to a richer set of benchmarks and algorithms. One issue that we need to address is scaling of $L^\#$ to bigger models. Our prototype implementation easily learns Mealy machines with hundreds of states, but fails to learn larger models such as the ESM benchmark of [57] (3410 states, 78 inputs) because the observation tree becomes too big ($\approx$25 million nodes will be required for the ESM). We see several ways to address this issue, e.g., pruning the observation tree, only keeping short ADSs to separate the basis states, storing parts of the tree on disk, distributing the tree over multiple processors (parallelizing the learning process), and using existing platforms for big graph processing [54].

Aslam et al. [9] report on experiments in which active learning techniques are applied to 202 industrial software components from ASML. Out of these, interface protocols could be successfully derived for 134 components (within a give time bound). One of the main conclusions of the study is that the equivalence checking phase (i.e. conformance testing of hypothesis models) is the bottleneck for scalability in industry. We believe that a tighter integration of learning and testing, as enabled by $L^\#$, will be key to address this challenging problem.

It will be interesting to extend $L^\#$ to richer frameworks such as register automata, symbolic automata and weighted automata. In fact, we discovered $L^\#$ while working on a grey-box learning algorithm for symbolic automata.

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