Automata Learning and Identification of the Support of Language Models

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Abstract

We study the learnability of languages in the *Next Symbol Prediction* (NSP) setting, where a learner receives only positive examples from a language together with, for every prefix, (i) whether the prefix itself is in the language and (ii) which next symbols can lead to an accepting string. This setting has been used in prior work to empirically analyze neural sequence models, and additionally, we observe that efficient algorithms for the NSP setting can be used to learn the (truncated) support of language models. We first show that the class of DFAs with at most n states is identifiable from positive examples augmented with these NSP labels. Nevertheless, even with this richer supervision, we show that PAC-learning DFAs remains computationally hard, and exact identification using only membership queries cannot be achieved in polynomial time. We then present $\mathrm{L}^\star_{\mathrm{nsp}}$, an extension of Angluin's $\mathrm{L}^\star$ algorithm, and show that DFAs can be PAC-learned efficiently using a language-model–based teacher that answers membership queries and generates valid strings conditioned on prefix prompts. Finally, we conduct a comprehensive empirical evaluation on 11 regular languages of varying complexity. Using $\mathrm{L}^\star_{\mathrm{nsp}}$, we extract DFAs from Transformer-based language models trained on regular languages to evaluate the algorithm's effectiveness and identify erroneous examples.

1 Introduction

Language models (LMs) are now deployed across text, vision, and bioinformatics; yet their internal computation and potential outputs they generate remain difficult to interpret. This motivates a basic question: given black-box access to a model, can we extract a compact, interpretable formal object, such as a deterministic finite automaton (DFA), that accepts (approximately) the same strings as those that lie in the model's generative support? We develop a formal framework for this problem and study its learnability in a setting that closely mirrors how LMs are typically used in practice.

We formalize and study the problem of learnability of languages in the *Next Symbol Prediction* (NSP) setting. Here, a learner receives only *positive* strings from a target language, together with rich supervision for every prefix: a membership bit indicating whether the prefix itself is in the language and a vector of "continuation" bits indicating which next symbols admit some accepting continuation. A prediction is correct only if the hypothesis matches *all* membership and continuation labels at *every* prefix of the example.

This setup has a natural interpretation in the context of language models: when decoding with top-p (Holtzman et al., 2020), top-k, or min-p (Minh et al., 2025) sampling, the per-prefix continuation set is precisely the set of admissible next tokens, and termination corresponds to allowing the end-of-sequence token. In particular, positive-only NSP supervision is naturally obtained from black-box models and avoids the need for inventing artificial distributions over negative strings; at the same time, the requirement for correct predictions at every prefix makes the task challenging. Figure 1 illustrates NSP labels on a Dyck example and how admissible-next-token sets can be read from a language model.

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Additionally, while NSP has been widely used to *evaluate* sequence models on formal-language benchmarks (see e.g. Bhattamishra et al. (2020a), Ebrahimi et al. (2020), Gers and Schmidhuber (2001), Suzgun et al. (2019) and references therein), the learnability of languages under NSP and its relationship to conventional binary classification has not been established.

Our contributions. We investigate the question of learnability in the NSP setting within the computational learning theory framework by studying computational complexity and oracle requirements. We also conduct a systematic empirical evaluation with several regular languages, using Transformer-based language models as teachers.

(i) Identifiability and hardness. We give a PAC-style formulation of learning using NSP labels and show that positive examples augmented with NSP labels are information-theoretically sufficient to identify minimal DFAs. Concretely, distinct minimal DFAs always disagree on the NSP labeling of some positive string, yielding finite teaching sets and a well-defined equivalence oracle in the NSP model. At the same time, we prove that NSP supervision does *not* remove the key *computational barriers* for learning regular languages. The key technical argument is a construction that renders all but one continuation label uninformative, allowing a reduction to well-known hardness results (Kearns and Valiant, 1994). Thus, even with the richer labels, efficient (improper) learning remains computationally intractable (under standard cryptographic assumptions). We further show that identification with membership queries alone cannot be achieved in polynomial time for certain natural DFA families, even when each query returns all NSP labels. Together, these results suggest that while NSP labels offer some benefit, they do not, in general, circumvent computational hardness.

(ii) Learning with a language-model teacher. Motivated by the hardness results, we study a more powerful, though still practically motivated, learning framework based on prefix-conditional generative queries. These can easily be simulated using black-box access to an LM. In addition to membership queries, the learner can issue *generative* queries that return positively labeled NSP strings conditioned on a *prefix* prompt. We extend Angluin's $\mathrm{L}^\star$ algorithm (Angluin, 1987) to design a new algorithm we denote $\mathrm{L}^\star_{\mathrm{nsp}}$, that uses membership and generative queries to construct a DFA consistent with the observed NSP labels. The guarantee is distribution-specific: $\mathrm{L}^\star_{\mathrm{nsp}}$ PAC-learns with respect to the distribution induced by the teacher language model. This perspective is aligned with our goal of identifying the model's (truncated) support and is particularly appealing in the context of generative models, where the target distribution over negative strings is either undefined or arbitrary. Conditional generation is both a natural capability of modern LMs and turns out to be a powerful query primitive for efficient learning in the NSP framework.

(iii) Empirical evaluation and analysis. We apply the $\mathrm{L}^\star_{\mathrm{nsp}}$ algorithm to extract DFAs from Transformer teachers trained on eleven regular languages of varying complexity, including the Tomita grammars, Parity, and bounded Dyck languages. We study how NSP accuracy, the number of extracted states, and runtime scale with the number of positive training strings. Across tasks, a modest amount of positive data with NSP labels typically suffices to recover the target automata or their teacher-support counterparts. When the teacher is imperfect (e.g., for Parity, Tomita-5), the extracted DFA reveals systematic errors by identifying strings in the symmetric difference between the target and the teacher's support. Ablations further indicate that the continuation labels are heavily used on languages with transitions to dead states (e.g., bounded Dyck), leading to improved sample complexity over binary labels alone. These experiments underscore a practical point: while NSP labels cannot break worst-case computational barriers, they are easy to obtain from modern sequence models and can be leveraged effectively in practice.

1.1 Related Work

Learnability of DFAs. Classical results show that inferring DFAs from labeled examples is computationally hard— finding the minimum consistent DFA is NP-hard (Angluin, 1978, Gold, 1978, Pitt and Warmuth, 1993), and even (improper) PAC learning is intractable under cryptographic assumptions (Kearns and Valiant, 1994). With queries and counterexamples, Angluin (1987) showed that regular languages are learnable in polynomial time. Under structural assumptions, several works have studied PAC learnability for probabilistic DFAs (Clark and Thollard, 2004, Palmer and Goldberg, 2007). The area remains active with recent theory on counterexample handling and lower bounds in the MAT framework (Kruger et al., 2023,

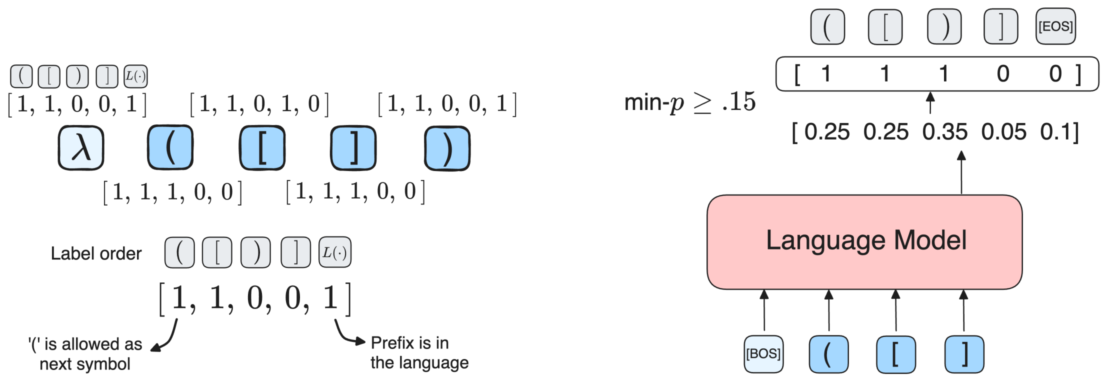


Figure 1: *Left:* An example of a string with NSP labels from the Dyck-2 language. The language consists of well-balanced parentheses with two types of brackets. *Right:* An illustration of how NSP labels can be obtained from a language model. See Section 2 for details.

Vaandrager et al., 2022). We build on this line of research by characterizing the learnability of DFAs in a new setting relevant to learning the support of language models, and by situating prior empirical analyses of neural nets in the appropriate context.

Automata extraction from neural models was introduced by Giles et al. (1992), Omlin and Giles (1996) and has been an active field (Muškardin et al., 2022, Wang et al., 2018). Notably, Weiss et al. (2018) developed a method for white-box extraction based on L⋆, and several subsequent works have focused on the extraction of weighted automata/PDFAs (Eyraud and Ayache, 2024, Wei et al., 2024, Weiss et al., 2019). Recent work (Zhang et al., 2024) has also explored L⋆-like methods for Transformer-based classifiers. Mayr et al. (2023) learn a PDFA abstraction of an LM via a distributional congruence. Our focus is on support identification, where we characterize learnability and conduct empirical analysis based on a new provable extension of the L⋆ algorithm.

2 Problem Definition

Notation. A deterministic finite automaton (DFA) is a tuple $A = (Q, \Sigma, \delta, q_0, F_A)$ with finite state set Q, alphabet Σ, transition function $\delta : Q \times \Sigma \to Q$, start state q_0, and a subset of accepting states $F_A \subseteq Q$. The language of A is $L_A \subseteq \Sigma^*$; write $A(x) = L_A(x) \in \{0,1\}$ and $|A|$ denotes the number of states $|Q|$. Fix an order $\Sigma = \{\sigma_1, \dots, \sigma_{|\Sigma|}\}$. For $x = w_1 \cdots w_N$, let the length-n prefix be $x_{:n} := w_1 \cdots w_n$ for $0 \le n \le N$. We use q_{dead} to denote a dead state with $q_{\text{dead}} \notin F_A$ and $\delta(q_{\text{dead}}, \sigma) = q_{\text{dead}}$ for all $\sigma \in \Sigma$ (unique, if present, in a minimal DFA). We use DFA_n to denote the class of DFAs with at most n states.

2.1 Next Symbol Prediction (NSP) Setting

For a language $L \subseteq \Sigma^*$ and any $x \in \Sigma^*, \sigma \in \Sigma$, define the *continuation bit*

$$\varphi_L(x, \sigma) \; := \; \mathbb{I}\Big[\, \exists s \in \Sigma^* \text{ s.t. } x \cdot \sigma \cdot s \in L \,\Big].$$

If L is regular with minimal DFA A, then with $q = \delta(q_0, x)$ we have $\varphi_A(x, \sigma) = 0$ if and only if $\delta(q, \sigma) = q_{\text{dead}}$. The continuation vector at q is defined as $\varphi_A(q) = [\varphi_A(q, \sigma_1), \dots, \varphi_A(q, \sigma_{|\Sigma|})] \in \{0,1\}^{|\Sigma|}$. For strings $x \in \Sigma^*$, write $\varphi_A(x) := \varphi_A(\delta(q_0, x))$ and $\varphi(x, \sigma) := \varphi(\delta(q_0, x), \sigma)$.

A positive NSP–labeled example is a string $x = w_1 \cdots w_N \in L$ together with, for every prefix $x_{:n}$ $(0 \le n \le N)$, its membership $L(x_{:n})$ and all continuation bits $(\varphi(x_{:n}, \sigma))_{\sigma \in \Sigma}$. We collect these as

$$f_L(x) \; := \; \Big((\varphi(x_{:n}, \sigma_i))_{i=1}^{|\Sigma|},\, L(x_{:n}) \Big)_{n=0}^{N} \in \{0,1\}^{(|\Sigma|+1)(N+1)}.$$

We will use the term NSP labels to refer to such labels (See Fig. 1, left for an illustration). We instantiate predictors via automata. For a DFA A define $f_A(x) := \Big((\varphi(x_{:n}, \sigma_i))_{i=1}^{|\Sigma|},\, L_A(x_{:n}) \Big)_{n=0}^{|x|}$. Let $f_{A^\star}$ denote the target NSP labeling function. The per-example loss is the $0/1$ sup-norm mismatch $\mathrm{err}(f_A(x), f_{A^\star}(x)) := \|f_A(x) - f_{A^\star}(x)\|_\infty = \mathbb{I}[f_A(x) \neq f_{A^\star}(x)]$, i.e., it equals 1 iff *any* membership/continuation label for any prefix is wrong; the NSP loss on $\mathcal{D}$ (supported on strings in $L_{A^\star}$) is $\mathcal{L}_{\mathrm{NSP}}(f_A; f_{A^\star}, \mathcal{D}) := \mathrm{E}_{x\sim\mathcal{D}}[\mathrm{err}(f_A(x), f_{A^\star}(x))]$. Because all $(|\Sigma|+1)(|x|+1)$ labels must be simultaneously correct, NSP is stringent in the sense that a naive random guesser has a near-zero chance of zero error on a typical example (contrast with $\approx$50% in binary classification).

2.2 Learning the Truncated Support of Language Models

For a vocabulary Σ containing [EOS], let a language model LM define next-token probabilities $p_{\mathrm{LM}}(\cdot \mid y)$ on Σ for each prefix $y \in \Sigma^*$. A sampling/truncation rule $\mathcal{T}$ (e.g., top-p, top-k, per-step min-p) maps y to the admissible next-symbol set $\mathcal{C}_{\mathcal{T}}(y) \subseteq \Sigma$, with $[\mathsf{EOS}] \in \mathcal{C}_{\mathcal{T}}(y)$ exactly when y may terminate (see Fig. 1, right for an illustration). The $\mathcal{T}$*-truncated support* of LM is the set of all strings that can be generated by running LM under $\mathcal{T}$. Formally,

$$L_{\mathrm{LM}}^{\mathcal{T}} := \Big\{ x = w_1 \cdots w_N :\ \forall\, 0 \le n < N,\ w_{n+1} \in \mathcal{C}_{\mathcal{T}}(w_1 \cdots w_n) \ \text{ and } \ [\mathsf{EOS}] \in \mathcal{C}_{\mathcal{T}}(x) \Big\}.$$

The NSP labelling oracle induced by the language model LM and truncation strategy $\mathcal{T}$ is then,

$$L_{\mathrm{LM}}^{\mathcal{T}}(y) := \mathbb{I}[[\mathsf{EOS}] \in \mathcal{C}_{\mathcal{T}}(y)], \qquad \varphi^{\mathcal{T}}(y, \sigma) := \mathbb{I}[\sigma \in \mathcal{C}_{\mathcal{T}}(y)] \ \ (\sigma \in \Sigma),$$

and we set $f_{\mathrm{LM}}^{\mathcal{T}}(x) := \Big((\varphi^{\mathcal{T}}(x_{:n}, \sigma_i))_{i=1}^{|\Sigma|},\, L_{\mathrm{LM}}^{\mathcal{T}}(x_{:n}) \Big)_{n=0}^{|x|}$. If generation under $\mathcal{T}$ terminates almost surely, then for any admissible step there exists a finite accepting continuation, so $\varphi^{\mathcal{T}}$ coincides with the global NSP semantics above.

From NSP learning to learning support. Let $\mathcal{D}_{\mathrm{LM}}^{\mathcal{T}}$ be the distribution of strings generated by LM under $\mathcal{T}$. Any PAC learner that, from NSP-labeled positive examples $(x, f^\star(x))$, outputs $\hat{f}$ with $\mathcal{L}_{\mathrm{NSP}}(\hat{f}; f^\star, \mathcal{D}) \le \epsilon$ immediately yields, by instantiating $f^\star = f_{\mathrm{LM}}^{\mathcal{T}}$ and $\mathcal{D} = \mathcal{D}_{\mathrm{LM}}^{\mathcal{T}}$, a procedure that learns the $\mathcal{T}$-truncated support of LM with NSP error at most ϵ.

Oracle simulation. With black-box access to LM and rule $\mathcal{T}$, one can simulate the typical example oracle $\mathrm{EX}(f_{\mathrm{LM}}^{\mathcal{T}}; \mathcal{D}_{\mathrm{LM}}^{\mathcal{T}})$ by sampling $x \sim \mathcal{D}_{\mathrm{LM}}^{\mathcal{T}}$ and returning $(x, f_{\mathrm{LM}}^{\mathcal{T}}(x))$. Membership queries can be computed by checking if a string takes an admissible path based on the truncation strategy $\mathcal{T}$ and if [EOS] is permissible at the last step.

3 Identifiability and Equivalence in the NSP setting

Before studying efficient learnability, it is first necessary to establish whether NSP labels are *necessary* and *sufficient*, in an information-theoretic sense, to identify a target language from positive examples alone. By *unique identification from positive* NSP *data* for a target DFA $A^\star$ with $L_{A^\star} \neq \emptyset$, we mean that there exists a finite set $S \subseteq L_{A^\star}$ such that

$$\forall A \in \mathrm{DFA}_n, \qquad \Big(\forall x \in S,\ f_A(x) = f_{A^\star}(x) \Big) \implies A \equiv A^\star. \tag{1}$$

Any such S will be called a (positive) NSP *teaching set* for $A^\star$.

Note that positive strings alone without additional labels are not sufficient for such identifiability: over $\Sigma = \{0,1\}$, let $L_A = \Sigma^*$ and $L_{A^\star} = 1^*$. Every positive example $x \in 1^*$ is accepted by both, so no positive counterexample exists. The same obstruction persists even if, in addition, the oracle reveals the *membership* *of each prefix*: for any $x \in 1^*$ and any prefix y of x we have $L_A(y) = L_{A^\star}(y) = 1$, so positive examples with prefix-membership labels still cannot distinguish A from $A^\star$. The key property of the NSP labels is that the continuation bits convey information about strings *not* in the language: $\varphi(y, \sigma) = 0$ certifies that no extension of $y\sigma$ is accepted. This additional information suffices to separate distinct minimal DFAs using positive examples only.

Proposition 3.1. *Let $A \neq A^\star$ be minimal DFAs with $L_{A^\star} \neq \emptyset$. Then there exists $x \in L_{A^\star}$ such that $f_A(x) \neq f_{A^\star}(x)$. Equivalently, the oracle $\mathrm{EQ}(A; A^\star)$ is well-defined: it either returns "equivalent" or a positive counterexample $(x, f_{A^\star}(x))$.*

The proof is in Appendix E.

Consequences. Proposition 3.1 has two immediate consequences. First, finite teaching sets exist: for each $A \in \mathrm{DFA}_n \setminus \{A^\star\}$, choose a witness $x_A \in L_{A^\star}$ with $f_A(x_A) \neq f_{A^\star}(x_A)$ guaranteed by the proposition, and set $S := \{x_A : A \in \mathrm{DFA}_n \setminus \{A^\star\}\} \subseteq L_{A^\star}$. Then S is a positive NSP teaching set for $A^\star$ in the sense of (1). Second, it also implies that the equivalence query oracle (cf. App. E) is well-defined in the NSP setting, which is crucial for exact learning to be feasible.

4 Hardness of Learning

We study efficient PAC learnability in the NSP setting. An algorithm $\mathcal{A}$ is an efficient PAC learner for a class $\mathcal{F}$ if for every $f \in \mathcal{F}$ and every distribution $\mathcal{D}$ supported on positive examples, $\mathcal{A}$ runs in polynomial time on NSP–labeled inputs and outputs $\hat{f}$ such that, with probability at least $1 - \delta$, $\mathcal{L}_{\mathrm{NSP}}(\hat{f}; f, \mathcal{D}) \leq \epsilon$.

Note that the continuation labels can be highly informative for certain classes. Consider *Conjunctions*: Boolean monomials $f : \{0,1\}^N \to \{0,1\}$, e.g., $f(z) = z_2 \wedge \bar{z}_4$. In the conventional classification model, learning Conjunctions is known to require $\Theta(N)$ labeled examples. In the NSP model, one positive example $x \in f^{-1}(1)$ suffices. For each prefix $x_{:k}$, the label $\varphi(x_{:k}, 0)$ equals 0 if and only if the literal z_{k+1} appears in the target; likewise, $\varphi(x_{:k}, 1) = 0$ if and only if the literal $\bar{z}_{k+1}$ appears. Thus, by reading the continuation labels across the N prefixes, the learner recovers exactly which literals are present and hence identifies the target monomial from a single positive NSP example. While the NSP labels may provide a statistical advantage for some classes, we show that in the general case, they are not enough to remove the computational barriers for learning DFAs.

We relate learnability in the NSP setting to standard PAC learning for acyclic DFAs that accept only strings of a fixed length. Throughout this section, we work over the binary alphabet $\Sigma = \{0, 1\}$.

Notation for classes. For $N \in \mathbb{N}$ and a polynomial $p(\cdot)$, define

$$\mathrm{ADFA}^N_{p(N)} := \Big\{ A : A \text{ is a DFA with at most } p(N) \text{ states and } L_A \subseteq \{0,1\}^N \Big\},$$

and write $\mathrm{ADFA}_{p(\cdot)} := \bigcup_{N \geq 1} \mathrm{ADFA}^N_{p(N)}$. As defined earlier, DFA_n denotes the class of DFAs with at most n states. Under the convention that the transition function is total, any minimal $A \in \mathrm{ADFA}^N_{p(N)}$ has a dead (sink) state with self-loops on both input symbols. If instead one allows a partial transition function δ, interpreting undefined transitions as implicit moves to a dead state, then the automata in $\mathrm{ADFA}^N_{p(N)}$ are acyclic in the usual sense.

Background. Kearns and Valiant (1994) show that, for a suitable polynomial p, weak PAC learning of $\mathrm{ADFA}_{p(\cdot)}$ in the conventional classification (binary-label) model is as hard as inverting certain cryptographic functions.

Theorem 4.1 (Kearns and Valiant (1994))**.** *There exists a polynomial $p(\cdot)$ such that the problems of inverting RSA, factoring Blum integers, etc., are probabilistic polynomial-time reducible to weakly learning $\mathrm{ADFA}_{p(\cdot)}$ in the standard PAC setting.*

We prove that an efficient PAC algorithm for $\mathrm{ADFA}^N_{p(N)}$ in the NSP setting would yield an efficient PAC algorithm for $\mathrm{ADFA}^N_{p(N)}$ in the conventional classification setting. Together with Theorem 4.1, this implies cryptographic hardness for NSP learning of these Boolean Acyclic DFAs and consequently the general class of DFAs.

Construction. The key technical idea is the construction in the following Lemma, where we construct from any $A \in \mathrm{ADFA}^N_{p(N)}$ a DFA $A^\oplus$ over length-N+1 inputs whose NSP labels are uninformative before depth N, while at depth N the continuation bit for symbol 0 recovers A's label. More precisely, we will construct a DFA $A^\oplus$ with at most $|A| + N + 1$ states such that: (i) the NSP labels of any prefix of length $< N$ will be $(1,1,0)$, and (ii) crucially, the NSP label for a string $u \in \Sigma^N$ of length N will be $(A(u), 1, 0)$. The ADFA $A^\oplus$ accepts all strings x of length $N + 1$ ending with 1 and some ending with 0 depending on $A(x_{:N}$. Thus, with respect to $A^\oplus$, predicting the first continuation bit (corresponding to symbol 0) is equivalent to predicting membership in L_A.

Lemma 4.2. *[Padded Construction] From a Boolean Acyclic DFA A we can construct, in time polynomial in $|A| + N$, a DFA $A^\oplus$ with $L_{A^\oplus} \subseteq \{0,1\}^{N+1}$ and*

$$\text{for } u \in \{0,1\}^N \text{ and } b \in \{0,1\} : \quad u \cdot b \in L_{A^\oplus} \iff \Big(A(u) = 1\Big) \text{ or } \Big(b = 1\Big). \tag{2}$$

Moreover, for every prefix y with $|y| < N$,

$$\Big(\varphi(y, 0),\ \varphi(y, 1),\ L_{A^\oplus}(y)\Big) = (1, 1, 0),$$

and for every $u \in \{0,1\}^N$,

$$\Big(\varphi(u, 0),\ \varphi(u, 1),\ L_{A^\oplus}(u)\Big) = \Big(A(u),\ 1,\ 0\Big).$$

The construction adds at most N+1 states.

See App. C.1 for the proof of the construction.

Reduction from standard learning to NSP learning. Let D be any distribution on $\{0,1\}^N$. Define the *padded* distribution $D^\oplus$ on $\{0,1\}^{N+1}$ by sampling $u \sim D$ and returning $x := u \cdot 1$. By (2), $x \in L_{A^\oplus}$ for every u, so $D^\oplus$ is supported on positive examples as required by the NSP setting. Moreover, given a labeled standard example (u, y) with $y = A(u)$, the full NSP label vector $f_{A^\oplus}(x)$ for $x = u \cdot 1$ is computable from (u, y):

$$\begin{aligned}
&\text{for } 0 \le \ell < N : \quad \Big(\varphi(x_{:\ell}, 0), \varphi(x_{:\ell}, 1), L(x_{:\ell})\Big) = (1, 1, 0),\\
&\text{for } \ell = N : \quad \Big(\varphi(x_{:N}, 0), \varphi(x_{:N}, 1), L(x_{:N})\Big) = (y, 1, 0),\\
&\text{for } \ell = N{+}1 : \quad \Big(\varphi(x_{:N+1}, 0), \varphi(x_{:N+1}, 1), L(x_{:N+1})\Big) = (0, 0, 1).
\end{aligned}$$

Here $x_{:\ell}$ denotes the length-ℓ prefix of the padded string x.

Theorem 4.3. *Fix N and a polynomial $p(\cdot)$. If $\mathrm{ADFA}^N_{p(N)}$ is efficiently PAC-learnable in the NSP setting from positive examples, then $\mathrm{ADFA}^N_{p(N)}$ is efficiently PAC-learnable in the conventional classification (binary-label) setting.*

Proof. Let $\mathcal{A}_{\mathrm{NSP}}$ be an efficient NSP learner for $\mathrm{ADFA}^N_{p(N)}$. From i.i.d. labeled samples $(u^{(i)}, y^{(i)})$ with $y^{(i)} = A(u^{(i)})$, form positive NSP examples $\Big(x^{(i)}, f_{A^\oplus}(x^{(i)})\Big)$ where $x^{(i)} = u^{(i)} \cdot 1$ using the rule above, and feed them to $\mathcal{A}_{\mathrm{NSP}}$. Let $\hat{f}$ be the returned predictor so that, with probability at least $1 - \delta$,

$$\mathcal{L}_{\mathrm{NSP}}\Big(\hat{f};\, f_{A^\oplus},\, D^\oplus\Big) = \mathop{\mathbb{E}}_{u \sim D}\Big[\mathbb{I}\Big[\hat{f}(u \cdot 1) \neq f_{A^\oplus}(u \cdot 1)\Big]\Big] \ \le\ \epsilon.$$

Define a standard classifier $h : \{0,1\}^N \to \{0,1\}$ by

$$h(u) \ :=\ \text{the bit predicted by } \hat{f} \text{ for } \varphi(x_{:N}, 0) \text{ on } x = u \cdot 1.$$

Whenever $\mathbb{I}\left[\hat{f}(x) = f_{A^\oplus}(x)\right] = 1$, Lemma 4.2 gives $h(u) = A(u)$. Therefore

$$\Pr_{u \sim D}\left[h(u) \neq A(u)\right] \;\le\; \Pr_{u \sim D}\left[\hat{f}(u \cdot 1) \neq f_{A^\oplus}(u \cdot 1)\right] \;\le\; \epsilon,$$

yielding an efficient PAC learner in the standard setting. The state complexity of $A^\oplus$ is at most $p(N) + N + 1$, preserving polynomial time complexity. □

Corollary 4.3.1 (Cryptographic hardness for NSP learning of acyclic DFAs)**.** *Under the assumptions of Theorem 4.1, there is no polynomial-time weak learner for* $\mathrm{ADFA}_{p(\cdot)}$ *in the* NSP *setting. Otherwise, Theorem 4.3 would yield a polynomial-time weak learner in the standard setting, contradicting Theorem 4.1.*

Discussion. The theorem shows that richer supervision via NSP does not circumvent the computational barrier for learning regular languages: under standard assumptions, there is no polynomial-time weak learner for $\mathrm{ADFA}_{p(\cdot)}$ and hence for DFAs even in the NSP setting. This remains true when the learner receives both positive and negative examples with NSP labels, showing that such additional supervision does not mitigate these barriers. The hardness is *improper*: it rules out efficient learning even when the hypothesis need not be a DFA, and thus applies to neural models trained to match NSP labels.

Learning with Membership Queries. In addition to passive examples, we also study *active* access in the NSP model. A conventional membership-query oracle $\mathrm{MQ} : \Sigma^* \to \{0,1\}$ takes an input string and returns whether it belongs to the target language. In the NSP setting, the oracle $\mathrm{MQ}_{\mathrm{nsp}}(x)$ returns the full vector of $(|\Sigma|+1)(|x|+1)$ labels for any $x \in \Sigma^*$. We show that certain simple classes known to be not identifiable in polynomial time with conventional queries become efficiently identifiable with $\mathrm{MQ}_{\mathrm{nsp}}$ with the help of additional labels. However, more generally, we show that some classes of DFAs and Boolean functions remain non-identifiable in polynomial time even with NSP labels from $\mathrm{MQ}_{\mathrm{nsp}}$. See App. D for details.

5 Learning with a Language Model Teacher

Given the hardness of learning with random examples or membership queries alone, we now study the learnability of DFAs in a relatively more powerful model based on the information one can conveniently obtain via blackbox access to language models such as neural sequence models or PDFAs.

Problem and Assumptions. Let LM be a language model which induces a distribution over strings $\mathcal{D}_{\mathrm{LM}}$ (correspondingly $\mathcal{D}_{\mathrm{LM}}^{\mathcal{T}}$ for a sampling strategy $\mathcal{T}$). Assume that the support of the distribution $\mathcal{D}_{\mathrm{LM}}$ is a regular language and let $A^\star$ be the DFA that recognizes the support $L_{A^\star}$. Given blackbox access to such a language model, we would like to find $\hat{A}$ such that $\Pr_{x \sim \mathcal{D}_{\mathrm{LM}}}\left[f_{\hat{A}}(x) \neq f_{A^\star}(x)\right] \le \epsilon$ with high probability. In this setting, a learner has access to two types of queries: *(i) Membership queries* $\mathrm{MQ}(x) \in \{0,1\}$ which return $A^\star(x)$, and *(ii) Generative queries* $\mathrm{Gen}_{\mathcal{D}_{\mathrm{LM}}}(\cdot)$ which take an input string or prompt x and generate a string s along with NSP labels based on the distribution $\mathcal{D}_{\mathrm{LM}}$ conditioned on the prompt x. Note that both these queries can be simulated with blackbox access to the language model (cf. App. F.2).

Approach. Broadly, we first sample a set X with m NSP-labeled examples from the distribution $\mathcal{D}_{\mathrm{LM}}$ using Generative queries $\mathrm{Gen}_{\mathcal{D}_{\mathrm{LM}}}(\lambda)$ where λ denotes the empty string. We will then use an extension of the $\mathrm{L}^\star$ algorithm to make use of the membership queries and generative queries to obtain a hypothesis DFA $\hat{A}$ in polynomial time such that $|\hat{A}| \le |A^\star|$ and $\hat{A}$ is *consistent* with the NSP labels of all m examples. A standard Occam-style generalization bound then yields a PAC-guarantee for the learning problem.

Preliminaries from $\mathrm{L}^\star$. We briefly recall the notions from $\mathrm{L}^\star$ (Angluin, 1987) based on modern treatments (Kearns and Vazirani, 1994) that we use in $\mathrm{L}^\star_{\mathrm{nsp}}$ (cf. App. F.1 for a more detailed description). The algorithm maintains finite sets $Q \subseteq \Sigma^*$ of *access words* and $T \subseteq \Sigma^*$ of *test words*, both containing the empty string λ. Intuitively, Q represents states and T represents distinguishing strings. With respect to a target language $L_{A^\star}$ and any ordering $t_1, \ldots, t_{|T|} \in T$, we can define a row vector of T-labels for any string x: $\mathrm{row}(x) = [L_{A^\star}(x \cdot t_1), \ldots, L_{A^\star}(x \cdot t_{|T|})] \in \{0,1\}^{|T|}$. The pair (Q, T) is defined to be *separable* with respect to language $L_{A^\star}$ if every row vector is unique: $\mathrm{row}(q) \neq \mathrm{row}(q')$ for $q, q' \in Q$. The pair (Q, T) is *closed* if for every

$q \in Q$ and $\sigma \in \Sigma$, there exists $q' \in Q$ such that $\text{row}(q \cdot \sigma) = \text{row}(q')$. When (Q, T) is closed and separable, one can construct a DFA hypothesis with state set Q and transitions based on T-labels (see App. F.1 for the construction). A crucial fact about this $\text{L}^\star$ framework is that (Lemma F.1) when (Q, T) is closed and separable with respect to language $L_{A^\star}$, then $|Q| \leq |A^\star|$ for the minimal DFA $A^\star$.

Given a set of labeled examples, $\text{L}^\star$ starts from $Q = T = \{\lambda\}$ and iteratively adds states and distinguishing strings based on label disagreements, maintaining a key invariant that (Q, T) remains separable. The procedure has two steps: (i) *Closure* (Lemma F.2): if (Q, T) is not closed, use membership queries to update (Q, T) to achieve closure in polynomial time. (ii) *Counterexample processing* (Lemma F.3): once closed, construct a hypothesis DFA $\hat{A}$ and find a *counterexample* x in the training set with $\hat{A}(x) \neq A^\star(x)$. Then, using at most $|x|$ membership queries, one can identify $q' \notin Q$ and $t' \notin T$ so that $(Q \cup \{q'\}, T \cup \{t'\})$ is separable. This step is the backbone of $\text{L}^\star$: membership disagreements can be used to obtain new access and test words to refine (Q, T).

In the NSP setting, counterexamples may arise from continuation-labels rather than membership disagreements, so Lemma F.3 does not apply as is. This is where $\text{L}^\star_{\text{nsp}}$ departs from $\text{L}^\star$: we use a different method to process counterexamples $x \in L_{A^\star}$ using continuation-label disagreements. The next lemma formalizes this update rule for $\text{L}^\star_{\text{nsp}}$.

Lemma 5.1. *Let (Q, T) be closed and separable, and let $\hat{A}$ be the minimal DFA induced by (Q, T). Suppose there exists a string x with $f_{\hat{A}}(x) \neq f_{A^\star}(x)$. Then one can find $q' \notin Q$ and $t' \notin T$ such that $(Q \cup \{q'\}, T \cup \{t'\})$ is separable, using membership queries and at most one generative query in polynomial time. If a generative query is used, let y denote its output; otherwise set $y = \lambda$. The total number of membership queries is at most $|x| + |y|$, and the running time is polynomial in $|x| + |y| + |Q|$.*

Proof. By definition, we have a string such that $A^\star(x) = 1$ and $f_{\hat{A}}(x) \neq f_{A^\star}(x)$. Thus, there is a prefix $x_{:n}$ of x at which the NSP labels disagree; the disagreement is either (a) in the *membership* label for $x_{:n}$, or (b) in one of the *continuation* labels for some symbol $\sigma \in \Sigma$. We treat these two cases separately. For all cases, our goal will be to construct a string x' such that we can invoke Lemma F.3 to obtain q' and t'.

Case A: Membership-label disagreement. There exists a prefix $x_{:n}$ of x such that $A^\star(x_{:n}) \neq \hat{A}(x_{:n})$. In this case we may simply take $x' = x_{:n}$ and apply Lemma F.3. That lemma produces an access word $q' \notin Q$ and a test word $t' \notin T$ in time polynomial in $|x'|$ (and using at most $|x'|$ membership queries), and it guarantees that $(Q \cup \{q'\}, T \cup \{t'\})$ is separable.

Case B: Continuation-label disagreement. There exists a prefix $x_{:n}$ of x and a symbol $\sigma \in \Sigma$ such that

$$\varphi_{\hat{A}}(x_{:n}, \sigma) \;\neq\; \varphi_{A^\star}(x_{:n}, \sigma).$$

We distinguish two subcases according to the value of the target continuation label.

Subcase B1: $\varphi_{A^\star}(x_{:n}, \sigma) = 0$ and $\varphi_{\hat{A}}(x_{:n}, \sigma) = 1$. By the semantics of the continuation labels for the target, $\varphi_{A^\star}(x_{:n}, \sigma) = 0$ means that for every suffix $s \in \Sigma^*$ we have $A^\star(x_{:n} \cdot \sigma \cdot s) = 0$. On the other hand, $\varphi_{\hat{A}}(x_{:n}, \sigma) = 1$ means that the state $\tilde{q} := \delta_{\hat{A}}(q_0, x_{:n} \cdot \sigma)$ that $\hat{A}$ reaches after traversing $x_{:n} \cdot \sigma$ is not the dead state.

Therefore, we can search within $\hat{A}$ from $\tilde{q}$ to see whether there is some accepting continuation. Run a breadth–first search in $\hat{A}$ starting at $\tilde{q}$; if the search reaches a final state $q \in F_{\hat{A}}$, let s' be a shortest suffix labeling such a path. Then by construction, the length $|s'| \leq |Q|$ and

$$A^\star(x_{:n} \cdot \sigma \cdot s') = 0 \qquad \text{and} \qquad \hat{A}(x_{:n} \cdot \sigma \cdot s') = 1,$$

so $x' := x_{:n} \cdot \sigma \cdot s'$ is a standard membership counterexample. Applying Lemma F.3 to x' yields $q' \notin Q$ and $t' \notin T$ in polynomial time.

Subcase B2: $\varphi_{A^\star}(x_{:n}, \sigma) = 1$ and $\varphi_{\hat{A}}(x_{:n}, \sigma) = 0$. The target label $\varphi_{A^\star}(x_{:n}, \sigma) = 1$ asserts that there exists a suffix $s' \in \Sigma^*$ with $A^\star(x_{:n} \cdot \sigma \cdot s') = 1$. In contrast, $\varphi_{\hat{A}}(x_{:n}, \sigma) = 0$ means that $\delta_{\hat{A}}(\delta_{\hat{A}}(q_0, x_{:n}), \sigma) = q_{\text{dead}}$, hence $\hat{A}(x_{:n} \cdot \sigma \cdot s) = 0$ for every suffix s.

As a consequence of Prop. D.1, we also have that such a suffix cannot be found in polynomial time using membership queries only. Thus, to find an accepting suffix, we call the generative query oracle with input

$x_{:n} \cdot \sigma$. Since $\varphi_{A^\star}(x_{:n}, \sigma) = 1$, such a suffix is guaranteed to exist. Let $s' = \mathrm{Gen}_{\mathcal{D}_{\mathrm{LM}}}(x_{:n} \cdot \sigma)$ and we have $x' = x_{:n} \cdot \sigma \cdot s'$ which is rejected by $\hat{A}$ (since it reaches a dead state after reading $x_{:n} \cdot \sigma$). Thus, invoking Lemma F.3 on x' produces the desired q' and t' in polynomial time.

In all cases we obtain $q' \notin Q$ and $t' \notin T$ such that $(Q \cup \{q'\}, T \cup \{t'\})$ is separable. This completes the proof. □

Algorithm. Given a set of m NSP-labeled examples, the $\mathrm{L}^\star_{\mathrm{nsp}}$ algorithm works as follows. It starts with $Q = T = \{\lambda\}$ and iteratively updates the pair (Q, T) such that they are always separable. For a hypothesis $\hat{A}$ associated with (Q, T), it finds the first disagreement in the NSP labels with the examples in the training set X. Using membership queries and generative queries based on Lemma 5.1, it updates the pair (Q, T) and adds at least one state whenever there is a disagreement with the training examples. The closure step remains the same as in the original $\mathrm{L}^\star$ algorithm. The algorithm terminates when $\hat{A}$ induced by (Q, T) is consistent with all the training examples. Since $|Q|$ is guaranteed to be at most $|A^\star|$, the algorithm must terminate after at most $|A^\star|$ disagreements with the training examples. A pseudocode of the $\mathrm{L}^\star_{\mathrm{nsp}}$ is given in Algorithm 1.

Theorem 5.2. *Let $A^\star$ be the minimal DFA that recognizes the support language $L_{A^\star} \subseteq \Sigma^*$ of the distribution $\mathcal{D}_{\mathrm{LM}}$. Given m NSP labelled examples $X = \langle x^{(i)}, f_{A^\star}(x^{(i)}) \rangle_{i=1}^m$, with access to membership query oracle MQ and generative query oracle $\mathrm{Gen}_{\mathcal{D}_{\mathrm{LM}}}$ with respect to $\mathcal{D}_{\mathrm{LM}}$, Algorithm 1 outputs a DFA $\hat{A}$ such that $f_{\hat{A}}(x^{(i)}) = f_{A^\star}(x^{(i)})$ for all $i = 1, \ldots, m$. The running time is polynomial in $|A^\star|, |\Sigma|, \max_i |x^{(i)}|$, and the length of the longest string returned by the generative query oracle.*

Proof. If the target language is $L_{A^\star} = \emptyset$, then the initial hypothesis DFA $\hat{A}$ at Line 6 will also be such that $\hat{A}(x) = 0$ for all $x \in \Sigma^*$. Whenever a disagreement with any training example is found, by Lemma 5.1, the algorithm will add at least one string to Q and effectively identify at least one new state from $A^\star$. By Lemma F.1, we have that $|Q| \leq |A^\star|$ and thus after at most $|A^\star|$ iterations of the main loop (Line 7) or equivalently, at most $|A^\star|$ calls to Lemma F.3, we have that $|Q| = |A^\star|$. Each state in Q is uniquely identified with a set of distinguishing strings that are consistent with $A^\star$. Since (Q, T) is closed and the transitions are defined using membership queries to check T-equivalence, the final DFA is isomorphic to the target DFA $A^\star$. Hence, in such a case $\hat{A} = A^\star$ and the hypothesis must be consistent with all training examples. Thus, it will terminate. The algorithm can, of course, terminate with $|Q| < |A^\star|$ if the hypothesis DFA is consistent with all the training examples.

□

As a consequence of the above theorem and the fact that $\log |\mathrm{DFA}_n| = O(n \log n)$ (Lemma B.3), Theorem 5.3 follows from standard Occam's razor arguments.

Theorem 5.3. *Let $A^\star \in \mathrm{DFA}_n$ be any minimal DFA with at most n states, and let $\mathcal{D}_{\mathrm{LM}}$ be a distribution over strings whose support is $L_{A^\star}$. There exists an algorithm with access to the membership query oracle MQ and generative query oracle $\mathrm{Gen}_{\mathcal{D}_{\mathrm{LM}}}$ producing NSP labeled examples in $L_{A^\star}$, that runs in time polynomial in $n, 1/\epsilon, 1/\delta$ and the length of the largest string produced by the generative query oracle, and with probability at least $1 - \delta$, outputs a DFA $\hat{A}$ such that,*

$$\mathcal{L}_{\mathrm{NSP}}(f_{\hat{A}}; f_{A^\star}, \mathcal{D}_{\mathrm{LM}}) = \Pr_{x \sim \mathcal{D}_{\mathrm{LM}}} \left[f_{\hat{A}}(x) \neq f_{A^\star}(x) \right] \leq \epsilon.$$

Discussion. A key benefit of this model of learning is that the guarantee we get is with respect to a desired distribution. For example, if one uses the $\mathrm{L}^\star$ algorithm to learn DFAs using positive and negative examples, the target distribution (on negative examples) is often unclear and can be artificial. In practice, for generative models, we often do not have access to the target distribution on *negative* examples. For the purpose of identifying the support of language models, arguably the most relevant distribution is the one induced by the model itself, e.g., if one intends to predict whether the language model will generate erroneous strings.

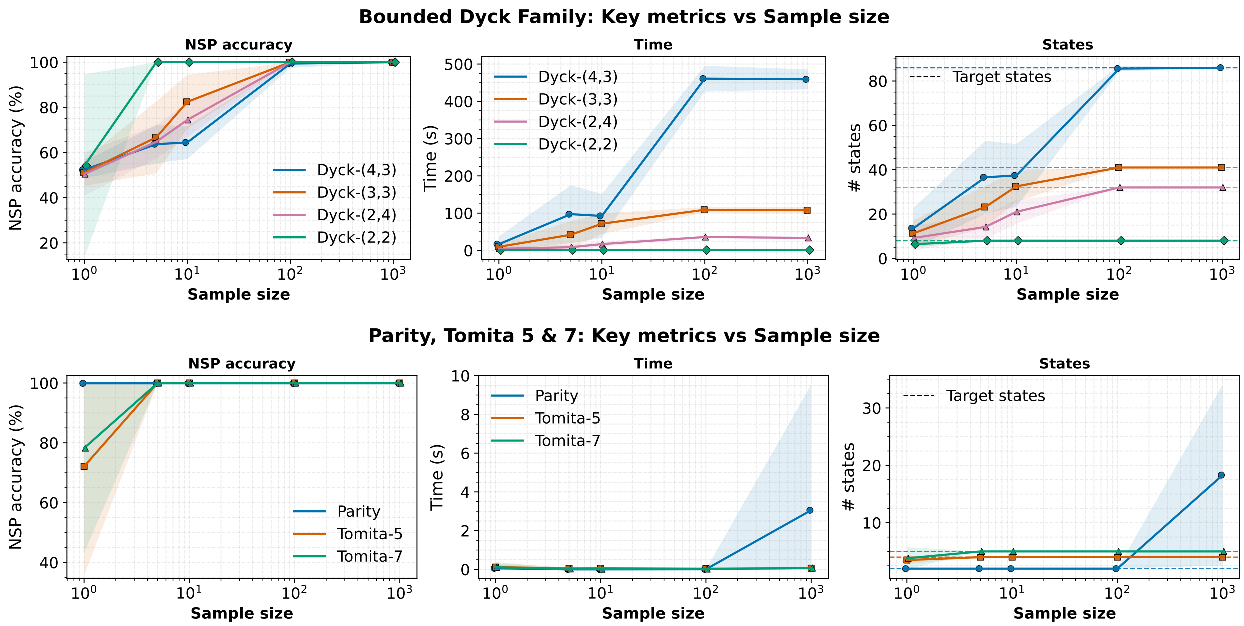


Figure 2: Key metrics for $L^\star_{\text{nsp}}$ across training-set sizes using a Transformer–LM teacher. Each point shows the mean over 10 trials; shaded regions denote standard deviation (see Sec. 6).

6 Empirical Analysis

We evaluate the $L^\star_{\text{nsp}}$ algorithm as a tool for extracting DFAs from Transformer language models trained on regular languages. Given NSP-labeled strings from the model, we study how the NSP error $\mathcal{L}_{\text{NSP}}$, the number of identified states, and the running time vary with the size of the training set. When the extracted automaton is not equivalent to the target DFA, we also find strings in the symmetric difference to identify *erroneous examples*. Further, we conduct ablations to analyze the effectiveness and usage of the continuation labels in the NSP setting.

Tasks. We consider 11 regular languages spanning 2–86 states: 6 Tomita grammars (Tomita, 1982), Parity, and 4 bounded Dyck languages. Tomita grammars comprise small DFAs (2–5 states) and are commonly used as a benchmark for automata extraction (Wang et al., 2018, Weiss et al., 2018, Zhang et al., 2024). Parity is the two-state language over $\Sigma = \{0, 1\}$ which contains all strings with an odd number of 1s. Bounded Dyck languages contain well-balanced parentheses up to a fixed depth and are regular. We denote by $\textsc{Dyck}\text{-}(n,k)$ the Dyck language with n bracket types and depth at most k. The depth of a Dyck string is the maximum number of unclosed brackets in any prefix of the string. These languages have a relatively larger number of states: $\sum_{i=0}^{k} n^i + 1$. We use four bounded Dyck instances: $\textsc{Dyck}\text{-}(2,2)$, $\textsc{Dyck}\text{-}(2,4)$, $\textsc{Dyck}\text{-}(3,3)$, and $\textsc{Dyck}\text{-}(4,3)$. Further details of the tasks are in App. G.

Setup. For each target language, we convert its canonical DFA to a PDFA to generate training strings. At non-final states, probability mass is split uniformly among transitions that avoid the dead state; at final states, generation terminates with probability t (otherwise, the next symbol is sampled as above). For each language, we choose t so that the empirical expected length is below 40.

Model training. We train Transformers as next-token predictors on sequences of the form [BOS] s_1 [EOS] s_2 [EOS] $\cdots$ with context window 250. Models use 8 layers and width 512, optimized with AdamW for up to 40k steps with early stopping. Our evaluation focuses on the support of the first string produced after [BOS]; the concatenated format matches standard training and provides additional learning signal.

DFA extraction. We use the trained Transformers to generate training sets of various sizes to evaluate the $L^\star_{\text{nsp}}$ algorithm. We create training sets with strings of length up to 80 that are generated and labeled using min-p sampling with threshold $p = 0.05$ as described in Sec. 2.2. The Transformer model serves as both

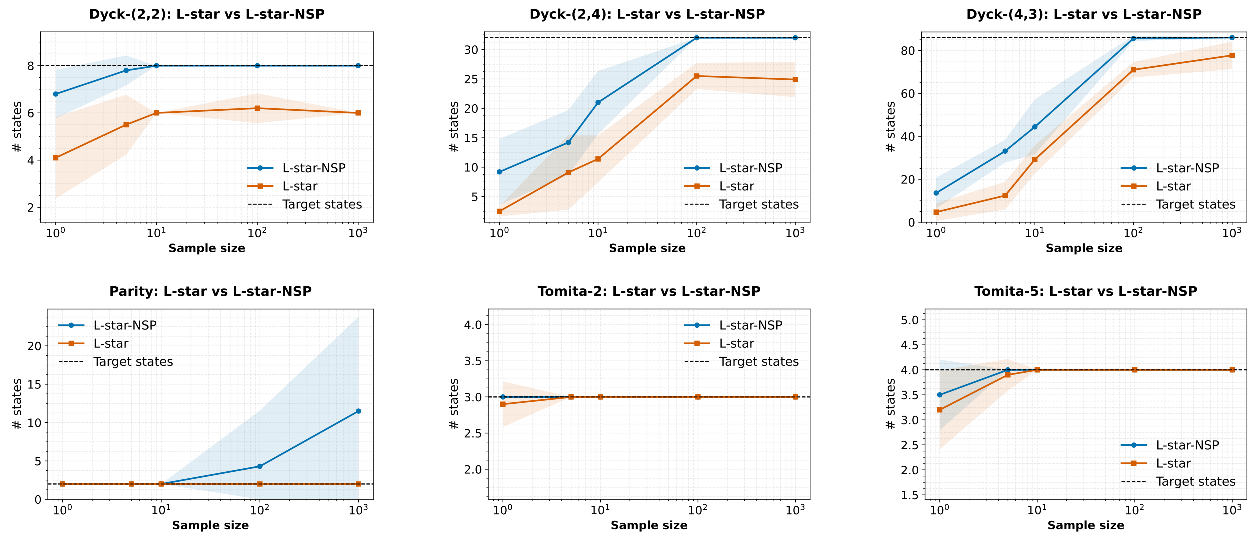


Figure 3: Comparison between binary labels (L*) and NSP labels (L$^\star_{\text{nsp}}$) by including negative examples by sampling from the untruncated distribution of the LM. Each point in the plots is the mean value over 10 trials; shaded regions show standard deviation. See Sec. 6 for details.

membership and generative query oracle for L$^\star_{\text{nsp}}$. We evaluate sample sizes $\{1, 5, 10, 100, 1000\}$; for each size, we run 10 independent trials and report means and standard deviations. For small targets (e.g., Tomita), even a single positive example can be informative.

Results. Figure 2 summarizes NSP accuracy, running time, and the number of extracted states for representative tasks. On Tomita, when teacher models are well trained, L$^\star_{\text{nsp}}$ recovers the target DFA quickly (often within a second; bottom row). For models that are not perfectly trained, such as for Parity, the algorithm extracts a much larger DFA and takes longer, depending on the number of target states. Note that since L$^\star_{\text{nsp}}$ adds a state only after finding a distinguishing string, the number of extracted states is always at most the number of states in the ground-truth DFA that recognizes the language model's support. Thus, even when we recover more states than the target DFA, the result is faithful to the language teacher's support.

Bounded Dyck languages have relatively much larger number of states (8–86 states). As shown in the top row of Figure 2, Dyck tasks naturally require more samples than Tomita, yet L$^\star_{\text{nsp}}$ converges to the target DFA and achieves near-perfect NSP accuracy within 100 examples. Our ablation experiments in App. G.4 indicate that the continuation labels are heavily used and play a crucial role in identifying the states of the target (see Table 3).

Identifying erroneous examples. When the learned DFA $\hat{A}$ is not equivalent to the target DFA $A^\star$, we construct the product DFA B which recognizes the strings in the symmetric difference of the two languages $L(B) = L(\hat{A}) \triangle L(A^\star)$. We use a BFS-like approach to identify several erroneous examples for the language model. Table 2 illustrates some erroneous examples for Bounded Dycks, Parity, and Tomita-5 language with LMs that weren't perfectly trained. Fig. 6 and 7 depict the extracted automaton for Parity and Tomita-5; the ones for DYCK-$(2, 2)$ and DYCK-$(3, 3)$ are too large to be visually informative. Note that these models were not intentionally trained to fail, and all the examples generated by the language models were in their respective target languages. The DFAs extracted by L$^\star_{\text{nsp}}$ were based on a few disagreements in the NSP labels of the generated strings. Training the language models for longer avoids such errors for synthetic languages of this scale. Note that the Transformer models used for Tomita-5 and Dyck languages in Figure 2 (well-trained) and Table 2 (imperfect) are different. See App. G.2 for further details.

NSP Label vs Binary Label Ablations. To assess the value of NSP labels, we compare binary labels (classical L*) with NSP labels (L$^\star_{\text{nsp}}$ extension) on six languages. We sample strings from the model's *untruncated* distribution (actual next-token probabilities) and label each as positive if it lies in the min-p truncated support $\mathcal{D}^{\mathcal{T}}_{\text{LM}}$ and negative otherwise. Naturally, most ($\approx 99.5\%$) samples are positive; nevertheless, even positive strings serve as counterexamples for $L^\star$ and using any natural variant of the distribution $\mathcal{D}_{\mathrm{LM}}$ will have few negative examples.

Results. Figure 3 plots the number of extracted states versus sample size (means over 10 runs). On bounded Dyck languages, $L^\star_{\mathrm{nsp}}$ reaches the target DFA with ≈ 10 examples for DYCK-$(2,2)$ and with ≈ 100 examples for DYCK-$(2,4)$ and DYCK-$(4,3)$, whereas $L^\star$ fails to recover the target even with 10^3 samples. For small Tomita DFAs, a single counterexample suffices, so both approaches perform similarly. For *Parity*, although the target DFA has 2 states, the teacher's support DFA is larger; with NSP labels, $L^\star_{\mathrm{nsp}}$ identifies this larger support (enabling the discovery of erroneous strings), while binary labels yield no disagreements and thus no additional states. Because almost all samples are positive, classification accuracy is uninformative; predicting 1 leads to near perfect accuracy and thus the extracted state count is the meaningful signal. Note that the claim here isn't that $L^\star_{\mathrm{nsp}}$ is superior (it is a direct extension of $L^\star$ itself). Rather, the goal here is to assess whether the additional labels are informative; the results indicate that leveraging NSP labels can be sample efficient for problems where the natural distribution primarily has positive examples.

7 Future Work and Limitations

A natural question that remains open is the efficient learnability of DFAs with membership (MQ) and equivalence queries (EQ) in the NSP setting. We show that with membership queries and two types of equivalence queries, DFAs are exactly learnable and discuss barriers to obtaining a standard MQ+EQ algorithm in App. F.3. Prop. 3.1 shows that NSP labels are sufficient and a teaching (or characteristic) set exists. However, the size of such a set obtained from Prop. 3.1 is likely to be quite loose and could possibly be improved.

Limitations. Even though the $L^\star_{\mathrm{nsp}}$ algorithm is polynomial-time, it inherits some of the limitations of the $L^\star$ framework it builds on, making it difficult to scale the approach to practical language models. In particular, when the target DFA (language model support) has a large number of states, the algorithm is quite slow. We observe that when models are poorly trained, the underlying DFA typically has thousands of states. The $L^\star_{\mathrm{nsp}}$ algorithm identifies about 1k states and the closure step is slow due to the $|Q||T||\Sigma|$ time complexity (discussed in more detail in App. G.3). Further, while the factor of $|\Sigma|$ may not play a significant role for synthetic languages, it has immediate consequences for language models trained on text that have a large vocabulary. An interesting future work would be to develop more efficient system-level improvements to speed up the algorithm to make it applicable to relatively more practical language models.

References

Dana Angluin. On the complexity of minimum inference of regular sets. *Information and control*, 39(3): 337–350, 1978.

Dana Angluin. Learning regular sets from queries and counterexamples. *Information and computation*, 75(2): 87–106, 1987.

Dana Angluin. Queries and concept learning. *Machine learning*, 2(4):319–342, 1988.

Satwik Bhattamishra, Kabir Ahuja, and Navin Goyal. On the Ability and Limitations of Transformers to Recognize Formal Languages. In *Proceedings of the 2020 Conference on Empirical Methods in Natural Language Processing (EMNLP)*, pages 7096–7116, Online, November 2020a. Association for Computational Linguistics. doi: 10.18653/v1/2020.emnlp-main.576. URL https://aclanthology.org/2020.emnlp-main.576.

Satwik Bhattamishra, Kabir Ahuja, and Navin Goyal. On the practical ability of recurrent neural networks to recognize hierarchical languages. In *Proceedings of the 28th International Conference on Computational Linguistics*, pages 1481–1494, Barcelona, Spain (Online), December 2020b. International Committee on Computational Linguistics. doi: 10.18653/v1/2020.coling-main.129. URL https://aclanthology.org/2020.coling-main.129.

Alexander Clark and Franck Thollard. Pac-learnability of probabilistic deterministic finite state automata. *Journal of Machine Learning Research*, 5(May):473–497, 2004.

Thomas Colcombet, Daniela Petrişan, and Riccardo Stabile. Learning Automata and Transducers: A Categorical Approach. In Christel Baier and Jean Goubault-Larrecq, editors, *29th EACSL Annual Conference on Computer Science Logic (CSL 2021)*, volume 183 of *Leibniz International Proceedings in Informatics (LIPIcs)*, pages 15:1–15:17, Dagstuhl, Germany, 2021. Schloss Dagstuhl – Leibniz-Zentrum für Informatik. ISBN 978-3-95977-175-7. doi: 10.4230/LIPIcs.CSL.2021.15. URL https://drops.dagstuhl.de/entities/document/10.4230/LIPIcs.CSL.2021.15.

Colin De la Higuera. *Grammatical inference: learning automata and grammars*. Cambridge University Press, 2010.

Javid Ebrahimi, Dhruv Gelda, and Wei Zhang. How can self-attention networks recognize Dyck-n languages? In Trevor Cohn, Yulan He, and Yang Liu, editors, *Findings of the Association for Computational Linguistics: EMNLP 2020*, pages 4301–4306, Online, November 2020. Association for Computational Linguistics. doi: 10.18653/v1/2020.findings-emnlp.384. URL https://aclanthology.org/2020.findings-emnlp.384/.

Rémi Eyraud and Stéphane Ayache. Distillation of weighted automata from recurrent neural networks using a spectral approach. *Machine Learning*, 113(5):3233–3266, 2024.

Felix A Gers and E Schmidhuber. Lstm recurrent networks learn simple context-free and context-sensitive languages. *IEEE Transactions on Neural Networks*, 12(6):1333–1340, 2001.

C Lee Giles, Clifford B Miller, Dong Chen, Hsing-Hen Chen, Guo-Zheng Sun, and Yee-Chun Lee. Learning and extracting finite state automata with second-order recurrent neural networks. *Neural Computation*, 4 (3):393–405, 1992.

E Mark Gold. Complexity of automaton identification from given data. *Information and control*, 37(3):302–320, 1978.

Michael Hahn. Theoretical limitations of self-attention in neural sequence models. *Transactions of the Association for Computational Linguistics*, 8:156–171, 2020.

Michael Hahn and Mark Rofin. Why are sensitive functions hard for transformers? In Lun-Wei Ku, Andre Martins, and Vivek Srikumar, editors, *Proceedings of the 62nd Annual Meeting of the Association for Computational Linguistics (Volume 1: Long Papers)*, pages 14973–15008, Bangkok, Thailand, August 2024. Association for Computational Linguistics. doi: 10.18653/v1/2024.acl-long.800. URL https://aclanthology.org/2024.acl-long.800/.

John Hewitt, Michael Hahn, Surya Ganguli, Percy Liang, and Christopher D. Manning. RNNs can generate bounded hierarchical languages with optimal memory. In Bonnie Webber, Trevor Cohn, Yulan He, and Yang Liu, editors, *Proceedings of the 2020 Conference on Empirical Methods in Natural Language Processing (EMNLP)*, pages 1978–2010, Online, November 2020. Association for Computational Linguistics. doi: 10.18653/v1/2020.emnlp-main.156. URL https://aclanthology.org/2020.emnlp-main.156/.

Ari Holtzman, Jan Buys, Li Du, Maxwell Forbes, and Yejin Choi. The curious case of neural text degeneration. In *International Conference on Learning Representations*, 2020. URL https://openreview.net/forum?id=rygGQyrFvH.

Michael Kearns and Leslie Valiant. Cryptographic limitations on learning boolean formulae and finite automata. *Journal of the ACM (JACM)*, 41(1):67–95, 1994.

Michael J Kearns and Umesh Vazirani. *An introduction to computational learning theory*. MIT press, 1994.

Loes Kruger, Bharat Garhewal, and Frits Vaandrager. Lower bounds for active automata learning. In François Coste, Faissal Ouardi, and Guillaume Rabusseau, editors, *Proceedings of 16th edition of the International Conference on Grammatical Inference*, volume 217 of *Proceedings of Machine Learning Research*, pages 157–180. PMLR, 10–13 Jul 2023. URL https://proceedings.mlr.press/v217/kruger23a.html.

Franz Mayr, Sergio Yovine, Matías Carrasco, Federico Pan, and Federico Vilensky. A congruence-based approach to active automata learning from neural language models. In François Coste, Faissal Ouardi, and Guillaume Rabusseau, editors, *Proceedings of 16th edition of the International Conference on Grammatical Inference*, volume 217 of *Proceedings of Machine Learning Research*, pages 250–264. PMLR, 10–13 Jul 2023. URL https://proceedings.mlr.press/v217/mayr23a.html.

Nguyen Nhat Minh, Andrew Baker, Clement Neo, Allen G Roush, Andreas Kirsch, and Ravid Shwartz-Ziv. Turning up the heat: Min-p sampling for creative and coherent LLM outputs. In *The Thirteenth International Conference on Learning Representations*, 2025. URL https://openreview.net/forum?id=FBkpCyujtS.

Edi Muškardin, Bernhard K Aichernig, Ingo Pill, and Martin Tappler. Learning finite state models from recurrent neural networks. In *International Conference on Integrated Formal Methods*, pages 229–248. Springer, 2022.

Christian W Omlin and C Lee Giles. Extraction of rules from discrete-time recurrent neural networks. *Neural networks*, 9(1):41–52, 1996.

Nick Palmer and Paul W Goldberg. Pac-learnability of probabilistic deterministic finite state automata in terms of variation distance. *Theoretical Computer Science*, 387(1):18–31, 2007.

Adam Paszke, Sam Gross, Francisco Massa, Adam Lerer, James Bradbury, Gregory Chanan, Trevor Killeen, Zeming Lin, Natalia Gimelshein, Luca Antiga, et al. Pytorch: An imperative style, high-performance deep learning library. *Advances in neural information processing systems*, 32, 2019.

Leonard Pitt and Manfred K Warmuth. The minimum consistent dfa problem cannot be approximated within any polynomial. *Journal of the ACM (JACM)*, 40(1):95–142, 1993.

Alec Radford, Jeff Wu, Rewon Child, David Luan, Dario Amodei, and Ilya Sutskever. Language models are unsupervised multitask learners. 2019.

Mirac Suzgun, Yonatan Belinkov, Stuart Shieber, and Sebastian Gehrmann. LSTM networks can perform dynamic counting. In *Proceedings of the Workshop on Deep Learning and Formal Languages: Building Bridges*, pages 44–54, Florence, August 2019. Association for Computational Linguistics. doi: 10.18653/v1/W19-3905. URL https://www.aclweb.org/anthology/W19-3905.

Masaru Tomita. Learning of construction of finite automata from examples using hill-climbing. rr: Regular set recognizer. Technical report, 1982.

Frits Vaandrager, Bharat Garhewal, Jurriaan Rot, and Thorsten Wißmann. A new approach for active automata learning based on apartness. In *International Conference on Tools and Algorithms for the Construction and Analysis of Systems*, pages 223–243. Springer, 2022.

Qinglong Wang, Kaixuan Zhang, Alexander G Ororbia II, Xinyu Xing, Xue Liu, and C Lee Giles. A comparative study of rule extraction for recurrent neural networks. *arXiv preprint arXiv:1801.05420*, 2018.

Zeming Wei, Xiyue Zhang, Yihao Zhang, and Meng Sun. Weighted automata extraction and explanation of recurrent neural networks for natural language tasks. *Journal of Logical and Algebraic Methods in Programming*, 136:100907, 2024.

Gail Weiss, Yoav Goldberg, and Eran Yahav. Extracting automata from recurrent neural networks using queries and counterexamples. In *International Conference on Machine Learning*, pages 5247–5256. PMLR, 2018.

Gail Weiss, Yoav Goldberg, and Eran Yahav. Learning deterministic weighted automata with queries and counterexamples. *Advances in Neural Information Processing Systems*, 32, 2019.

Thomas Wolf, Lysandre Debut, Victor Sanh, Julien Chaumond, Clement Delangue, Anthony Moi, Pierric Cistac, Tim Rault, Rémi Louf, Morgan Funtowicz, et al. Transformers: State-of-the-art natural language processing. In *Proceedings of the 2020 conference on empirical methods in natural language processing: system demonstrations*, pages 38–45, 2020.

James Worrell. Exactly learning regular languages using membership and equivalence queries. https://www.cs.ox.ac.uk/people/james.worrell/DFA-learning.pdf, 2018. Lecture notes, Computational Learning Theory, Oxford.

Yihao Zhang, Zeming Wei, and Meng Sun. Automata extraction from transformers. *arXiv preprint arXiv:2406.05564*, 2024.

Contents

Usage of Large Language Models

We used publicly available AI tools (LLMs) to improve the flow and clarity of the text in various places. LLMs were used to rephrase certain text to polish it and/or make it more concise. AI tools have also aided in writing the code for the experiments in the paper.

A FAQs

(1) *If $\mathrm{L}^{\star}_{\mathrm{nsp}}$ is an efficient polynomial time algorithm, why shouldn't we directly apply it to large language models (LLMs) to obtain a DFA that captures their support?*

There are a few nontrivial obstacles to directly applying the algorithm to LLMs. Firstly, the target language for an LLM could have a huge number of states, and currently, it is difficult to use the algorithm for targets beyond the order of a few thousand states. Secondly, while the complexity of the algorithm is polynomial, it still scales linearly with the size of the vocabulary, and LLMs have vocabularies that are in the order of tens of thousands. Lastly, the support of LLMs may not be regular, which could violate the main assumption, and the guarantees need not apply. We believe this work makes progress towards the larger goal of capturing the support of language models, but it is practically limited, similar to other existing methods for automata extraction.

(2) *To identify erroneous examples, can we not sample from a language model several times and then check if any of them are incorrect?*

In theory, one can sample repeatedly to identify erroneous strings in the support. We argue that better algorithms for this problem can make the identification of erroneous strings much more efficient. For instance, for the parity language, sampling 1k strings from a seemingly well-trained model does not seem to produce any erroneous examples. However, the DFA extracted by leveraging NSP labels provides us with numerous erroneous examples. We found that $\mathrm{L}^\star_{\mathrm{nsp}}$ could extract a DFA within 10 seconds using 1k generations from the language model, which could then be used to produce about 1k erroneous strings within 16 seconds (see App G.2 for details). While the current approach isn't scalable beyond such synthetic problems, further improvements could help make progress in more efficient identification of DFAs and, consequently, identification of erroneous examples.

(3) *On what kind of problems is it more beneficial to use* $\mathrm{L}^\star_{\mathrm{nsp}}$ *as opposed to directly using* $\mathrm{L}^\star$*?*

$\mathrm{L}^\star_{\mathrm{nsp}}$ is a direct extension of $\mathrm{L}^\star$ that exploits NSP labels when available. It can be more sample-efficient in positive-only or highly imbalanced settings typical of generative models. Empirically, on bounded Dyck languages, $\mathrm{L}^\star_{\mathrm{nsp}}$ recovered the target DFA with ≈10–100 examples, whereas without NSP labels, $\mathrm{L}^\star$ did not with 10^3 samples (Fig. 3); ablations also show the algorithm heavily uses continuation labels on Dyck tasks and some Tomita grammars (see Table 3 and Sec. G.4).

(4) *Does the hardness result imply that learning with random examples alone will likely fail?*

One should take note that the hardness results are generally for the worst-case setting. It is helpful to gain a formal understanding of the strengths and weaknesses of a problem but they do not immediately imply that learning will fail most of the times. The result indicates that efficient distribution-independent PAC-learning algorithms are not feasible under standard cryptographic assumptions. However, in practice, using scalable heuristic-based methods is often effective. Our goal was to characterize the learnability in the NSP setting to understand the power of the additional supervision available in the NSP setting and it implies that they are not powerful enough to mitigate certain computational barriers.

B Preliminaries

We define Probabilistic DFAs (PDFAs) formally here. Our result on learning with membership and generative queries (Theorem 5.3) has direct implications on learning the support of PDFAs. We also use PDFAs to generate strings for training Transformer language models.

Probabilistic DFAs (PDFAs). A probabilistic DFA is a DFA equipped with a stochastic emission rule. Formally, a PDFA is a tuple

$$\mathcal{P} = (Q, \Sigma, \delta, q_0, F, \pi),$$

where $(Q, \Sigma, \delta, q_0, F)$ is a DFA and, for each $q \in Q$, $\pi(\cdot \mid q)$ is a probability distribution on $\Sigma \cup \{\texttt{[EOS]}\}$ where $\texttt{[EOS]}$ denotes the termination symbol. At state q, the generator samples $w \in \Sigma \cup \{\texttt{[EOS]}\}$ according to $\pi(\cdot \mid q)$; if $w \in \Sigma$ the next state is $\delta(q, w)$, and if $w = \texttt{[EOS]}$ the sequence terminates. We say a string $x = w_1 \cdots w_N \in \Sigma^*$ is in the *support* of $\mathcal{P}$ if

$$\pi(w_1 \mid q_0) \cdot \pi(w_2 \mid \delta(q_0, w_1)) \cdots \pi(w_N \mid \delta(q_0, x_{:N-1}))\pi(\texttt{[EOS]} \mid \delta(q_0, x)) > 0.$$

The DFA that accepts exactly this support is the *support DFA* of $\mathcal{P}$.

NSP labels from PDFAs. In a PDFA $\mathcal{P}$, the NSP labels coincide with positivity of the local emission probabilities:

$$\varphi(y, \sigma) = \mathbb{I}\{\pi(\sigma \mid \delta(q_0, y)) > 0\}, \qquad L(y) = \mathbb{I}\{\pi(\texttt{[EOS]} \mid \delta(q_0, y)) > 0\}.$$

Thus, the NSP labelling oracle exposes exactly the admissible next symbols and termination at each prefix; for a PDFA this recovers the (untruncated) support of $\mathcal{P}$.

The following is an elementary but fundamental fact about minimal DFAs due to the Myhill-Nerode Theorem that is at the heart of many of our proofs and constructions.

Lemma B.1 (DFA basic fact)**.** *Let A be a minimal DFA recognizing L_A. For any two distinct strings $x, y \in \Sigma^*$, if there exists a suffix $s \in \Sigma^*$ such that $L_A(x \cdot s) \neq L_A(y \cdot s)$ then the strings x and y lead to two distinct states in the DFA A, i.e., $\delta_A(q_0, x) \neq \delta_A(q_0, y)$. If no such suffix exists, then they lead to the same state $\delta_A(q_0, x) = \delta_A(q_0, y)$.*

In a minimal DFA, distinct states are pairwise distinguishable by some continuation; conversely, strings with indistinguishable residual languages must reach the same state. This is the Myhill–Nerode characterization of minimality.

Lemma B.2. *Let the dead state q_{dead} be a state such that $q_{\text{dead}} \notin F$ and $\delta(q_{\text{dead}}, \sigma) = q_{\text{dead}}$ for all $\sigma \in \Sigma$. Then, a minimal DFA has at most one dead state.*

Assume there are two dead states. Since every suffix from a dead state is rejected, there cannot be a suffix that is accepted by one state and rejected by another. Further, by definition, both of them are non-final. Hence, they are Myhill–Nerode equivalent and must be merged in a minimal DFA.

Lemma B.3. *Let DFA_n be the class of DFAs over a fixed alphabet Σ with at most n states. Then $\log |\text{DFA}_n| = \mathcal{O}(n \log n)$.*

This is a well-known result (De la Higuera, 2010). The proof follows from the fact that for a DFA with at most n states, there are $n^{|\Sigma| \cdot n}$ and each state can either be an accept or reject state adds a factor of 2^n, and one of the states can be an initial state. Hence, the total number of possible DFAs is $2^n \cdot n^{|\Sigma| \cdot n + 1}$. Thus, $\log |\text{DFA}_n| = \mathcal{O}(n \log n)$.

C Hardness of Learning with Examples

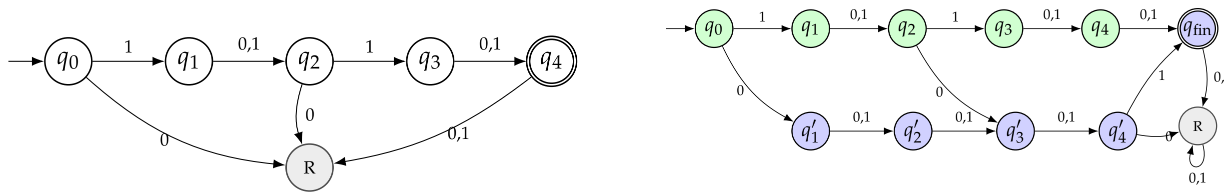
C.1 Proof Details: Boolean Acyclic DFAs

Fix $N \geq 1$ and a target DFA $A = (Q, \Sigma, \delta, q_0, F)$ with $L_A \subseteq \{0,1\}^N$. We first record a basic structural property of *minimal* DFAs for fixed-length languages.

Lemma C.1 (Unique depth in minimal $\text{ADFA}^N_{p(N)}$)**.** *If A is minimal and $L_A \subseteq \{0,1\}^N$, then every state $q \in Q \setminus \{q_{\text{dead}}\}$ is reachable by strings of exactly one length $\ell(q) \in \{0, 1, \ldots, N\}$. Consequently, every transition increases depth by one: if $\delta(q, \sigma) = q'$ with $q \neq q_{\text{dead}}$ and $q' \neq q_{\text{dead}}$, then $\ell(q') = \ell(q) + 1$. Acceptance occurs only at depth N.*

Proof. Let $q \in Q \setminus \{q_{\text{dead}}\}$ be reachable both by a string of length ℓ and by a string of length ℓ' with $\ell < \ell'$. The residual language at q is $R(q) := \{ s \in \Sigma^* : \delta(q, s) \in F \}$. If q is reached after ℓ symbols, then every $s \in R(q)$ must have length exactly $N - \ell$; if q is reached after ℓ' symbols, then every $s \in R(q)$ must have length exactly $N - \ell'$. Since $N - \ell \neq N - \ell'$, these sets are disjoint; hence $R(q)$ must be empty, contradicting $q \neq q_{\text{dead}}$ in a minimal DFA. Thus, each non-dead state has a unique depth $\ell(q)$. Any transition consumes one symbol, so $\ell(q') \leq \ell(q) + 1$; equality must hold by uniqueness of depth. Finally, if $q \in F$ had $\ell(q) \neq N$, then L_A would contain strings of length other than N, contrary to the assumption. $\square$

By Lemma C.1, we may index non-dead states by their unique depth $\ell(q) \in \{0, \ldots, N\}$ (the dead state has no depth).



(a) DFA for $z_1 \wedge z_3$, $x \in \{0,1\}^4$.

(b) Transformed DFA $(z_1 \wedge z_3) \vee z_5$, $x \in \{0,1\}^5$.

Figure 4: Transformation from Section C.1. In (b), green states are from the original DFA; blue states $q'_1, \ldots, q'_4$ ensure every prefix of length $< N$ has continuation labels $[1,1,0]$, and q'_4 routes to accept on input 1 (to the dead state on 0).

Lemma 4.2. *[Padded Construction] From a Boolean Acyclic DFA A we can construct, in time polynomial in $|A| + N$, a DFA $A^{\oplus}$ with $L_{A^{\oplus}} \subseteq \{0,1\}^{N+1}$ and*

$$\text{for } u \in \{0,1\}^N \text{ and } b \in \{0,1\}: \quad u \cdot b \in L_{A^{\oplus}} \iff \Big(A(u) = 1\Big) \text{ or } \Big(b = 1\Big). \tag{2}$$

Moreover, for every prefix y with $|y| < N$,

$$\Big(\varphi(y,0),\ \varphi(y,1),\ L_{A^{\oplus}}(y)\Big) = (1,1,0),$$

and for every $u \in \{0,1\}^N$,

$$\Big(\varphi(u,0),\ \varphi(u,1),\ L_{A^{\oplus}}(u)\Big) = \Big(A(u),\, 1,\, 0\Big).$$

The construction adds at most $N{+}1$ states.

Proof. Minimize the DFA A if it is not minimal. Create new states $q'_1, \ldots, q'_N$ and a new accepting state q_{fin}. For $1 \le i < N$ set

$$\delta_{A^{\oplus}}(q'_i, 0) = q'_{i+1}, \qquad \delta_{A^{\oplus}}(q'_i, 1) = q'_{i+1},$$

and at $i = N$ set

$$\delta_{A^{\oplus}}(q'_N, 1) = q_{\text{fin}}, \qquad \delta_{A^{\oplus}}(q'_N, 0) = q_{\text{dead}}.$$

From q_{fin} send both symbols to q_{dead} (so acceptance occurs only at length $N{+}1$).

Now modify A to create $A^{\oplus}$ as follows. For each non-dead state q with $\ell(q) < N$ and each $\sigma \in \{0,1\}$:

- If $\delta_A(q,\sigma) = q_{\text{dead}}$ in A, set $\delta_{A^{\oplus}}(q,\sigma) = q'_{\ell(q)+1}$ (redirect the dead transition into the chain).
- Otherwise set $\delta_{A^{\oplus}}(q,\sigma) = \delta_A(q,\sigma)$.

For each state q at depth N set

$$\delta_{A^{\oplus}}(q,1) = q_{\text{fin}}, \qquad \delta_{A^{\oplus}}(q,0) = \begin{cases} q_{\text{fin}}, & q \in F_A, \\ q_{\text{dead}}, & q \notin F_A. \end{cases}$$

See Figure 4 for a simple example construction for a Boolean Acyclic DFA computing a conjunction.

All transitions out of q_{dead} point to q_{dead}, i.e., $\delta_{A^{\oplus}}(q_{\text{dead}}, \sigma) = q_{\text{dead}}$ for both symbols. (If A recognizes the empty language, then $Q = \{q_{\text{dead}}\}$; in this case we additionally introduce a fresh start state $\tilde{q}_0$ of depth 0 with $\delta_{A^{\oplus}}(\tilde{q}_0, 0) = \delta_{A^{\oplus}}(\tilde{q}_0, 1) = q'_1$ and take $\tilde{q}_0$ as the start state; the conclusions below still hold.)

By construction, acceptance can occur only at q_{fin} after exactly $N{+}1$ symbols, so $L_{A^{\oplus}} \subseteq \{0,1\}^{N+1}$. The rule at depth N gives (2). For any prefix y with $|y| < N$, either an original transition still has an accepting continuation, or a dead transition is redirected to the chain $q'_{|y|+1} \to \cdots \to q'_N \to q_{\text{fin}}$ (taking the last symbol

1). Hence $\varphi(y,0) = \varphi(y,1) = 1$ and $L_{A^\oplus}(y) = 0$ for any y with $|y| < N$. At depth N, for every $u \in \{0,1\}^N$ our construction enforces

$$\delta_{A^\oplus}\Big(\delta_{A^\oplus}(q_0,u),1\Big) = q_{\text{fin}} \quad \text{and} \quad \delta_{A^\oplus}\Big(\delta_{A^\oplus}(q_0,u),0\Big) = \begin{cases} q_{\text{fin}}, & \delta_A(q_0,u) \in F_A, \\ q_{\text{dead}}, & \delta_A(q_0,u) \notin F_A, \end{cases}$$

so $\varphi(u,1) = 1$, $\varphi(u,0) = A(u)$, and $L_{A^\oplus}(u) = 0$, which is exactly

$$\Big(\varphi(u,0),\ \varphi(u,1),\ L_{A^\oplus}(u)\Big) = \Big(A(u),\ 1,\ 0\Big).$$

□

C.2 Boolean formulas

Exactly the same padding idea applies to Boolean formulas. Let F be any class of formulas $f : \{0,1\}^N \to \{0,1\}$ and define

$$f'(z_1,\ldots,z_{N+1}) \ := \ f(z_1,\ldots,z_L) \ \vee \ z_{N+1}.$$

Given a labeled standard example (u,y) with $y = f(u)$, set $x := u \cdot 1$. The NSP labels for the positive string x under f' are then computable from (u,y):

$$\text{for } \ell < N: \ (1,1,0), \qquad \text{for } \ell = N: \ (y,1,0), \qquad \text{for } \ell = N{+}1: \ (0,0,1),$$

with the same ordering (continuations first, then membership) as in §2. Thus an efficient NSP learner for $F' := \{f' : f \in F\}$ yields, by reading the depth-N continuation bit for symbol 0, an efficient PAC learner for F in the standard setting. In particular, cryptographic hardness results for learning formulas (e.g., via NC^1) carry over to the NSP setting by this reduction.

D Hardness of Learning with Membership Queries Only

Definition. A conventional membership query oracle $\mathrm{MQ} : \Sigma^* \to \{0,1\}$ takes an input string and returns whether it belongs to the target language or not. In the NSP setting, the membership query oracle $\mathrm{MQ}_{\mathrm{nsp}} : \Sigma^* \to \{0,1\}^{(|\Sigma|+1)(|x|+1)}$ returns all the NSP labels for an input string x. Since it contains the membership label of the input in its label, it has strictly more information than the conventional MQ oracle.

To understand how additional labels could provide more information, consider the following. If for any pair of prefixes or strings x, y, the $|\Sigma|$ continuation labels $\varphi(x), \varphi(y)$ differ, then it implies that they lead to two distinct states in the target DFA. This is because disagreement in the continuation label implies that there exists a suffix s such that $L(x \cdot s) \neq L(y \cdot s)$ and by Lemma B.1, they must lead to two different states.

There are some classes of functions that can be efficiently identified by $\mathrm{MQ}_{\mathrm{nsp}}$ but not by conventional MQ. For instance, consider the class of singleton Boolean functions $\mathcal{F}_1$ over $\{0,1\}^N$ which contains 2^N functions that accept exactly 'one' Boolean input of length N. Such functions cannot be identified with a polynomial number of conventional membership queries (see Angluin (1988) for a general characterization). The main idea is that no matter which input in $\{0,1\}^N$ a learner queries, an adversary can decide to always return 0 as the label until the learner queries $2^N - 1$ inputs.

Learning Singletons with $\mathrm{MQ}_{\mathrm{nsp}}$. The membership query oracle in the NSP setting is more powerful in the sense that such singleton Boolean functions can be identified easily in polynomial time. To see how, consider the following procedure: Let $x^\star \in \{0,1\}^N$ be the only string accepted by the target $f^\star : \{0,1\}^N \to \{0,1\}$. A learner first queries $\mathrm{MQ}_{\mathrm{nsp}}(x)$ any $x \in \{0,1\}^N$ and checks the $|\Sigma|$ continuation labels for the first index corresponding to the empty prefix λ. That indicates the first bit in the string accepted by the target function. Let $x_1^\star$ be the first bit of the target string. The learner then queries any string starting with $x_1^\star$ and obtains the second bit. Similarly, it can iteratively query $\mathrm{MQ}_{\mathrm{nsp}}$ and obtain the string $x^\star$ with at most N $\mathrm{MQ}_{\mathrm{nsp}}$ queries.

While the membership query oracle in the NSP setting $\mathrm{MQ}_{\mathrm{nsp}}$ is strictly more powerful than the one in the conventional classification setting, we show that there are DFAs in the class DFA_n that cannot be efficiently identified with membership queries only in the NSP setting. Similar to the case of hardness of learning with DFAs, we will construct functions where the NSP labels are uninformative and the problem becomes as hard as learning with the conventional membership query oracle.

Suffix Language family. Consider the following family of languages. Let $\Sigma = \{0, 1\}$ (the argument applies to any Σ with $|\Sigma| \geq 2$). Let $S = \{0, 1\}^{N/2}$ be the set of Boolean strings of length exactly $N/2$. The suffix language family $\mathcal{L}_S$ contains $2^{N/2}$ languages, where for each $s \in \{0, 1\}^{N/2}$, the language $L_s \in \mathcal{L}_S$ only accepts strings which end with the suffix s.

Each of the language $L_s \in \mathcal{L}_S$ can be represented by a DFA of size at most $N/2 + 1$. For any suffix or string s, create a state corresponding to each prefix of $s = s_0 \cdot s_1 \cdots s_{N/2}$ including the empty prefix $s_0 = \lambda$ which serves as the start state. Define transitions $\delta(s_{:k}, s_{k+1}) = s_{:k+1}$. For every other transition, if the symbol is s_1, then they go to the state $s_{:1}$ or else they go to s_0. From the first state, the shortest string that leads to the accept state is of length $N/2$. For every other state q_i in $q_1, \ldots, q_{N/2}$, the shortest accepting suffix is of length $\frac{N}{2} - i$.

Proposition D.1. *The class of Suffix languages $\mathcal{L}_S$ cannot be identified in polynomial time with membership queries $\mathrm{MQ}_{\mathrm{nsp}}$ in the* NSP *setting.*

Proof. A key characteristic of any of suffix language L_s is that, an accepting string exists for any prefix x. For any string x, the string $x \cdot s$ is in the language L_S. Thus, the continuation label for any prefix of any string will always be $(\varphi(x, 0), \varphi(x, 1)) = (1, 1)$. Hence, the continuation labels are not informative. The only informative signals are the membership labels.

In the NSP setting, the oracle $\mathrm{MQ}_{\mathrm{nsp}}$ will provide the membership labels of every prefix. Suppose a learner makes m $\mathrm{MQ}_{\mathrm{nsp}}$ queries where the maximum length of the queried input strings is k. Then each query eliminates at most $(k + 1) - \frac{N}{2} \leq k$ suffixes out of $2^{N/2}$ possible suffixes if all the membership labels are 0. Thus, in the worst case, the learner can eliminate at most $O(mk)$ suffixes or functions from the class. If both the number of queries m and input length k are polynomial in N, then they cannot identify the target s. Hence, either the number of queries must be exponential or the learner must use exponential computational steps. $\square$

Since the suffix language with suffixes of size $n/2$ can be represented with DFAs with at most n states, Prop. D.1 immediately implies that the class DFA_n cannot be identified in polynomial time with membership queries alone in the NSP setting even with the richer set of labels.

Boolean functions and Acyclic DFAs. A similar argument applies to the class of Boolean functions as well. Consider the class of functions $\mathcal{F}_{2^N - 1}$ over $\{0, 1\}^N$ which accept all bit strings of length N except one. It is straightforward to see that every function in that class can also be represented by Boolean Acyclic DFAs with exactly $N + 2$ states.

For such a class, the continuation labels will be unhelpful for all but one prefix of length $N - 1$. The same line of argument as earlier shows that each membership query can eliminate at most 1 function from the class. An adversary can decide to return membership labels 1 for every input query and choose the function based on the inputs queried by the learner, and hence in the worst case, the learner must make $2^{N-1} - 1$ queries before it can identify the target functions.

This implies that certain classes of Boolean functions, as well as the class ADFA_n cannot be identified with a polynomial number of $\mathrm{MQ}_{\mathrm{nsp}}$ queries in the NSP setting.

E Equivalence Queries and Identifiability

Let $\hat{A}$ and $A^\star$ be a hypothesis and target DFA, respectively. In the NSP setting, a valid Equivalence Query oracle $\mathrm{EQ}^+_{\mathrm{nsp}}(\hat{A}; A^\star)$ with respect to target $A^\star$ should take a hypothesis $\hat{A}$ as input and output 'equivalent' if $L_{\hat{A}} = L_{A^\star}$ or else it should return a counterexample $x \in L^\star_A$ such that $f_{\hat{A}}(x) \neq f_{A^\star}(x)$. In other words, the counterexample is a string that is accepted by the target DFA $A^\star$ but disagrees with $\hat{A}$ on at least one of the NSP labels.

Since the Equivalence query oracle can only produce strings accepted by $A^\star$, it is not immediately clear whether a counterexample will always exist when $L_{\hat{A}} \neq L_{A^\star}$. We show that positive examples with NSP labels are sufficient in the sense that for any pair of DFAs $\hat{A}, A^\star$ such that $L_{A^\star} \neq \emptyset$, there is always a counterexample if $L_{\hat{A}} \neq L_{A^\star}$. The following result is crucial for exact learning of DFAs with membership and equivalence queries to be feasible.

Proposition 3.1. *Let $A \neq A^\star$ be minimal DFAs with $L_{A^\star} \neq \emptyset$. Then there exists $x \in L_{A^\star}$ such that $f_A(x) \neq f_{A^\star}(x)$. Equivalently, the oracle $\mathrm{EQ}(A; A^\star)$ is well-defined: it either returns "equivalent" or a positive counterexample $(x, f_{A^\star}(x))$.*

Proof. Since $A \neq A^\star$, there exists a string $z \in \Sigma^*$ with $A(z) \neq A^\star(z)$. If $A^\star(z) = 1$, we may take $x = z$; the NSP vectors then disagree in the membership coordinate for the full prefix z, so $f_A(x) \neq f_{A^\star}(x)$ and we are done. Thus assume

$$A(z) = 1 \quad \text{and} \quad A^\star(z) = 0,$$

and let $q' = \delta_{A^\star}(q_0, z)$ be the state that the DFA $A^\star$ reaches after traversing the string z. We distinguish two possibilities for q'.

Case (i): $q' \neq q_{\text{dead}}$. Because $A^\star$ is minimal, any non-accepting state distinct from the dead state has an accepting continuation (otherwise it would be equivalent to q_{dead} and hence identified with it by minimality). Hence there exists a suffix $s \in \Sigma^*$ such that $A^\star(z \cdot s) = 1$.

Let $x := z \cdot s$. In the NSP label sequence for x, the membership coordinate at the prefix z is

$$L_A(z) = 1 \quad \text{and} \quad L_{A^\star}(z) = 0,$$

so $f_A(x) \neq f_{A^\star}(x)$. The oracle may therefore return this positive example x together with $f_{A^\star}(x)$.

Case (ii): $q' = q_{\text{dead}}$. Write $z = w_1 \cdots w_N$ with $w_i \in \Sigma$ and set $z_{:i} := w_1 \cdots w_i$ for $0 \leq i \leq N$ (with $z_{:0} = \lambda$). There exists an index $i \in \{0, \ldots, N-1\}$ such that

$$\delta_{A^\star}(q_0, z_{:i}) \neq q_{\text{dead}} \qquad \text{and} \qquad \delta_{A^\star}(q_0, z_{:i+1}) = q_{\text{dead}}. \tag{3}$$

$A^\star(z) = 0$ and the DFA $A^\star$ ends at q_{dead} after traversing z, so select the first position at which q_{dead} is entered. By minimality (as in Case (i)), the non-dead state $\delta_{A^\star}(q_0, z_{:i})$ admits an accepting continuation; hence there exists a suffix $s \in \Sigma^*$ with $A^\star(z_{:i} \cdot s) = 1$.

For the continuation bit at the prefix $z_{:i}$ and the next symbol w_{i+1}, (3) implies

$$\varphi_{A^\star}(z_{:i}, w_{i+1}) = 0.$$

On the other hand, since $A(z) = 1$ and $z = z_{:i}\, w_{i+1}\, (w_{i+2} \cdots w_N)$, there exists a suffix (namely $w_{i+2} \cdots w_N$) witnessing that

$$\varphi_A(z_{:i}, w_{i+1}) = 1.$$

Now set $x := z_{:i} \cdot s$. This x is accepted by $A^\star$, and the two NSP labelings disagree at the continuation coordinate $(z_{:i}, w_{i+1})$: $f_A(x) \neq f_{A^\star}(x)$.

Thus x is a valid counterexample for the oracle.

In either case, there exists a positive example x (accepted by $A^\star$) with $f_A(x) \neq f_{A^\star}(x)$ and if no such counterexample exists, then $A = A^\star$. □

F Learning with Membership and Generative Queries

F.1 L-star Preliminaries

We will first discuss the preliminaries of the L* framework based on modern and minimal treatments (Colcombet et al., 2021, Kearns and Vazirani, 1994).

Let $\hat{A}$ be a hypothesis DFA constructed by a learner and let $A^\star$ be the target DFA. We will refer to a string x such that $\hat{A}(x) \neq A^\star(x)$ as a *counterexample* that is provided by an Equivalence query oracle or by disagreement with an example in a training set.

Access and Test words. In this setup, we will have a pair of sets (Q, T) where $Q \subseteq \Sigma^*$ is a set of *access words*, and $T \subseteq \Sigma^*$ is a set of *test words*. Both Q and T are always nonempty. Intuitively, the set Q will play the role of states, where it will have a string corresponding to every state of our DFA. The test words T act as distinguishing strings for the access words Q. Both the sets Q, T contain the empty string λ. We will now define the notion of T-equivalence.

Definition F.1 (T-Equivalence)**.** For a non-empty set $T \subseteq \Sigma^*$ and a language L, two strings u, v are T-equivalent: $u \equiv_T v$, if for every string $s \in T$, the string $u \cdot s \in L$ if and only if $v \cdot s \in L$.

Closed and Separable. A pair (Q, T) is *closed* if for every access word $q \in Q$ and every symbol $\sigma \in \Sigma$, there exists an access word $q' \in Q$ such that $q \cdot \sigma \equiv_T q'$. A pair (Q, T) is defined to be *separable* if every two distinct access words $q, q' \in Q$ are not T-equivalent: $q \not\equiv_T q'$.

Constructing a DFA. Given a closed and separable pair (Q, T) and access to membership queries MQ, one can construct a DFA as follows.

- Set the $q_0 = \lambda \in Q$.
- For every $q \in Q$, add them to the set of accept states F if $\mathrm{MQ}(q) = 1$.
- For any access word q and symbol $\sigma \in \Sigma$, let q' be the word such that $q \cdot \sigma \equiv_T q'$. Then set the transition $\delta(q, \sigma) = q'$. Since (Q, T) is closed, such a state or access word q' must exist, and separability implies uniqueness of such a word.

To prove the correctness of our algorithm, we use the following technical lemmas from L* without proof.

Lemma F.1 (L* Fact (Angluin, 1987))**.** *Let (Q, T) be a closed and separable pair of sets which is consistent with some language L. Let $A^\star$ be the minimal automaton that decides L. Then, $|Q| \leq |A^\star|$.*

The above Lemma follows directly from Lemma B.1 and the fact that we have distinguishing string in T for each pair of strings in Q.

Lemma F.2 (L* Fact (Angluin, 1987))**.** *Let (Q, T) be a pair that is separable but not closed. Then, using at most $|Q||T|(|\Sigma| + 1)$ membership queries, and in time polynomial in $(|Q|, |T|, |\Sigma|)$, we can identify $q' \notin Q$, such that $(Q \cup \{q'\}, T)$ is separable.*

The following lemma is the crux of the original L* algorithm in terms of how it updates the pair (Q, T) based on disagreement between the hypothesis DFA and a labelled example.

Lemma F.3 (L* Fact (Angluin, 1987))**.** *Let (Q, T) be a closed and separable pair, and $\hat{A}$ be the associated DFA. Suppose $x \in \Sigma^*$ be a string such that $\hat{A}(x) \neq A^\star(x)$. Then using at most $|x|$ membership queries and in time polynomial in $|x|$, we can identify $q' \notin Q$ and $t' \notin T$ such that $(Q \cup \{q'\}, T \cup \{t'\})$ is separable.*

See Worrell (2018) for a tutorial of L* in the framework described here and the proofs of the precise Lemmas above.

F.2 Simulating Membership and Generative Queries

We describe how membership and generative queries can be conveniently simulated by blackbox access to the target language model LM. For a neural language model, the empty string corresponds to [BOS] token.

(i) *Membership Queries.* Given a query string $x = w_1 \cdots w_N \in \Sigma^*$, compute the NSP continuation labels for every prefix of x using the language model including the empty string λ. For a neural language model, this is simply done by obtaining the next token probabilities for each prefix and applying the truncation rule $\mathcal{T}$

Algorithm 1 $\mathrm{L}^{\star}_{\mathrm{nsp}}$ algorithm

$Q \leftarrow \{\lambda\}, \quad T \leftarrow \{\lambda\}$
$X = \langle x^{(i)}, f_{A^\star}(x^{(i)}) \rangle_{i=1}^{m}$ ▷ call $\mathrm{Gen}_{\mathcal{D}_{\mathrm{LM}}}(\lambda)$ m times
while (Q, T) not closed **do**
  Use Lemma F.2 to obtain q'; $Q \leftarrow Q \cup \{q'\}$
end while
Construct hypothesis automaton $\hat{A}$ from (Q, T)
while $\hat{A}$ not consistent with X **do**
  Choose $x \in X$ with $f_{\hat{A}}(x) \neq f_{A^\star}(x)$
  while $f_{\hat{A}}(x) \neq f_{A^\star}(x)$ **do** ▷ Use Lemma 5.1
    Let $x_{:n}$ be the prefix with first NSP mismatch
    let σ denote the symbol if it is a continuation mismatch
    if membership mismatch at $x_{:n}$ **then** ▷ Case A
      $w' \leftarrow x_{:n}$
    else if continuation mismatch with $A^\star$ forbids and $\hat{A}$ admits **then** ▷ Case B1
      $s' \leftarrow$ find $\hat{A}$-accepting suffix from $x_{:n} \cdot \sigma$
      $w' \leftarrow x_{:n} \cdot \sigma \cdot s'$
    else ▷ Case B2
      $w' \leftarrow x_{:n} \cdot \sigma \cdot \mathrm{Gen}_{\mathcal{D}_{\mathrm{LM}}}(x_{:n} \cdot \sigma)$
    end if
    Use Lemma F.3 on w' to obtain q' and t'
    $Q \leftarrow Q \cup \{q'\}$, $T \leftarrow T \cup \{t'\}$
    while (Q, T) not closed **do**
      Use Lemma F.2 to obtain q'; $Q \leftarrow Q \cup \{q'\}$
    end while
    Reconstruct $\hat{A}$ from (Q, T)
  end while
end while

(cf. Sec. 2.2). If for any prefix the continuation label $\varphi(x_{:n}, w_{n+1}) = 0$ then w_{n+1} is not a valid continuation so the oracle can return 0. If the path traversed by $w_1, \cdots, w_N$ is valid, then we can check whether $\varphi(x, [\mathsf{EOS}])$ is 1 or 0 and thus $\mathrm{MQ}(x) = \varphi(x, [\mathsf{EOS}])$.

(ii) *Generative Queries.* For any string or prefix x, the Generative Query Oracle $\mathrm{Gen}_{\mathcal{D}_{\mathrm{LM}}}(x)$ provides $(s, \boldsymbol{y})$ where s is a string from the distribution $\mathcal{D}^{\mathcal{T}}_{\mathrm{LM}}$ conditioned x. If no such continuation exists and x is at a dead state, then it returns 'None'. To simulate the example oracle or equivalently, to obtain examples from the target distribution $\mathcal{D}^{\mathcal{T}}_{\mathrm{LM}}$, one can simply query the oracle with empty string $\mathrm{Gen}_{\mathcal{D}_{\mathrm{LM}}}(\lambda)$. To obtain a continuation for a particular prefix x, one can provide it as an input prompt to the language model and first check whether x traverses a valid path based on the NSP labels as described above. If it does not then return 'None'. If it does then, then iteratively sample the next tokens using the truncation rule until the [EOS] is permissible $\varphi(x \cdot s, [\mathsf{EOS}]) = 1$.

F.3 On Exact Learning with Membership and Equivalence Queries

We show that the class of DFAs can be learned exactly with membership queries and *two types* of equivalence queries. (i) $\mathrm{EQ}^{+}_{\mathrm{nsp}}(A; A^\star)$ which returns a positive NSP-labelled counterexample with at least one disagreement in NSP labels or else it returns equivalence; (ii) $\mathrm{EQ}_{\mathrm{pos}}(A; A^\star)$ which just returns a string with no additional labels, such that the string is accepted by $A^\star$ but rejected by A if there exists such a string, otherwise it returns none. The problem of learning with just membership and NSP equivalence queries remains open.

For the setting where a learner has access to two types of equivalence queries, the algorithm is almost the same as the one described earlier (Alg. 1) with a couple of differences. Similar to the previous algorithm with

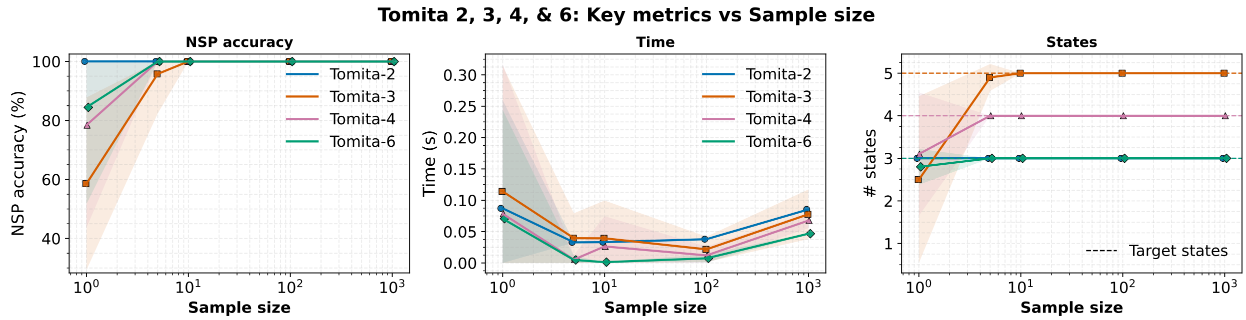


Figure 5: Key metrics for $L^\star_{\text{nsp}}$ on other Tomita grammars. See Sec. 6 for details.

membership and generative queries, the learner will maintain a pair (Q, T) and iteratively update them, but with counterexamples from EQ_{nsp} instead of a set of labelled examples. There are only two changes to address, which we describe below.

(i) The first thing to note is that by Proposition 3.1, the equivalence query oracle EQ^+_{nsp} is well-defined and always guaranteed to return a counterexample. If the target DFA $A^\star$ is such that $L_{A^\star} = \emptyset$, then the initial hypothesis DFA in Line 6 of Alg. 1 will be the same as $A^\star$ and thus, we do not need any counterexample.

(ii) Secondly, we do not have access to a generative query oracle anymore, so we cannot use it to find an accepting continuation when the target NSP label says that a suffix exists, but for our hypothesis DFA, no such suffix exists. The difficulty is that EQ^+_{nsp} against our hypothesis need not return a counterexample beginning with the particular prefix $x_{:n} \cdot \sigma$. To force such a witness, we will use $\text{EQ}_{\text{pos}}(A, A^\star)$. Consider the DFA $A_{x_{:n}\sigma}$ whose language is

$$L_{A_{x_{:n}\sigma}} := \Sigma^* \setminus \left(x_{:n} \cdot \sigma \cdot \Sigma^*\right),$$

i.e., $A_{x_{:n}\sigma}$ accepts exactly the strings that do *not* begin with the prefix $x_{:n} \cdot \sigma$. Submit the equivalence query $\text{EQ}_{\text{pos}}(A_{x_{:n}\sigma}; A^\star)$. Because $\varphi_{A^\star}(x_{:n}, \sigma) = 1$, there exists an accepted string with prefix $x_{:n} \cdot \sigma$; therefore, the oracle must return a positive counterexample of the form

$$x' = x_{:n} \cdot \sigma \cdot s' \quad \text{with} \quad A^\star(x') = 1.$$

But x' is rejected by $\hat{A}$ (the run reaches the dead state after reading $x_{:n} \cdot \sigma$), so x' is again a standard membership counterexample.

It is unclear whether exact learning with just membership and the NSP equivalence queries is feasible and is left as an open problem. When the learner gets a counterexample such that the only disagreement is of the form that $\varphi_{A^\star}(x_{:n}, \sigma) = 1$ and $\varphi_{\hat{A}}(x_{:n}, \sigma) = 0$, then one might wonder if a continuation can be recovered using the NSP membership query oracle MQ_{nsp} which provides additional label. But as a consequence of Prop. D.1, such an accepting continuation cannot be found in polynomial time using MQ_{nsp} only.

Table 1: Tomita grammars and descriptions.

Tomita grammar	Description
Tomita 1	Strings of only 1s (including the empty string), 1^*.
Tomita 2	Repeated "10" pattern, $(10)^*$.
Tomita 3	Any block with an *odd* number of consecutive 1s is always followed by a block with an *even* number of consecutive 0s.
Tomita 4	Strings that do not contain `000` as a substring.
Tomita 5	Strings with an even number of 0s and an even number of 1s.
Tomita 6	Strings where the difference between the number of 0s and the number of 1s is a multiple of 3.
Tomita 7	$0^*1^*0^*1^*$ (zero or more 0s, then 1s, then 0s, then 1s).

G Additional Ablations and Details of Experiments

We discuss additional details of the experimental setup as well as additional results for DFA extraction from language models.

G.1 Additional Details of the Setup

Tasks. We provide additional details about the tasks considered in our experiments.

Tomita grammars. Table 1 provides the description of the 7 Tomita grammars (Tomita, 1982) in the benchmark. We use all of them except the first one since it is trivial (1^*) and the results are uninformative. All the regular languages in the Tomita benchmark have 2-5 states. These benchmarks have primarily been used to extract DFAs from RNN or Transformer-based classifiers (Wang et al., 2018, Weiss et al., 2018, Zhang et al., 2024).

Parity. The Parity language is a simple two-state DFA recognizing whether the number of 1s in a string is odd or even. This task has been widely studied in the context of Transformers, and previous works have shown empirical (Bhattamishra et al., 2020a) and theoretical (Hahn, 2020, Hahn and Rofin, 2024) evidence to indicate that such functions are difficult for Transformers to model.

Bounded Dycks. DYCK-(n, k) represents the language with well-balanced parentheses with n types of brackets and depth at most k. These languages have also been widely used in analysis of sequence models (Bhattamishra et al., 2020b, Hewitt et al., 2020) since they capture hierarchical dependencies prevalent in natural languages. These DFAs have relatively larger number of states than Tomita grammars and Parity, and hence provide a testbed to evaluate learning algorithms on languages with increasing state complexity. We use the following languages in our experiments: DYCK-$(2, 2)$: 8 states, DYCK-$(2, 4)$: 32 states, DYCK-$(3, 3)$: 41 states, and DYCK-$(4, 3)$: 86 states.

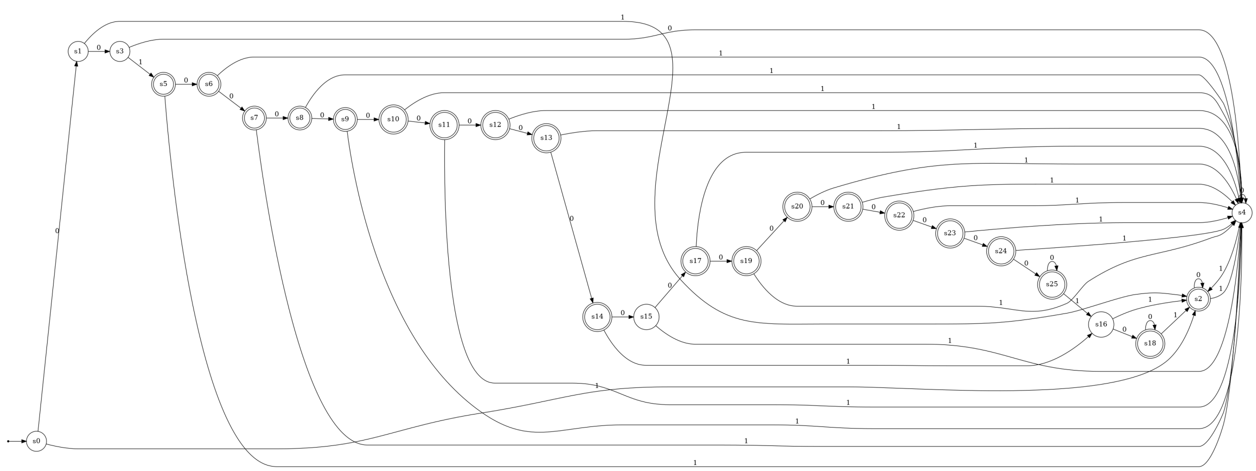


Figure 6: DFA with 26 states extracted by $\mathrm{L}^{\star}_{\text{nsp}}$ from Transformer trained on Parity. See App. G.2 for more details.

Compute. The experiments in the paper are not compute heavy. All our experiments were conducted using 8 NVIDIA Tesla V100 GPUs, each with 16GB of memory for training language models. Each run for up to 40k steps could take 1-6 hours depending on the task. Some runs are much shorter if the model achieves high accuracy quite early. The execution of $\mathrm{L}^{\star}_{\text{nsp}}$ is primarily on CPU, and uses the GPU to answer Generative and Membership queries with the Transformer language model. The time taken for each run of $\mathrm{L}^{\star}_{\text{nsp}}$ is provided in the main plots (Fig. 2 and 5). All of our implementations for language models in PyTorch (Paszke et al., 2019). For our experiments with Transformers, we use the Huggingface Transformers library (Wolf et al., 2020) with the GPT-2 (Radford et al., 2019) backbone.

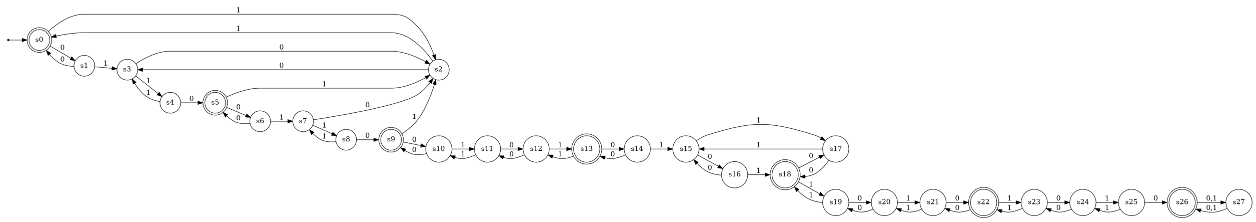


Figure 7: DFA with 28 states extracted by $\mathrm{L}^{\star}_{\mathrm{nsp}}$ from Transformer trained on Tomita-5. See App. G.2 for more details.

G.2 Identifying Erroneous Examples

When the Transformer models trained on regular languages are not perfect, the extracted DFA is not isomorphic to the target DFA used to generate training data for Transformers.

There are two key things to note about this event. (i) When the extracted DFA has more states than the target DFA (such as for Parity in Fig. 2), then it implies that the support language for Transformer has at least as many states as the extracted DFA. This is because states are always created after identifying distinguishing strings (Lemma B.1) using the teacher model. (ii) The cases where models are not perfectly trained and our extracted DFA identifies erroneous strings, the models are still well-trained in the sense that all 1k strings generated using the language model are in the target language. Thus, the difference comes from disagreement in some NSP label which the $\mathrm{L}^{\star}_{\mathrm{nsp}}$ algorithm then leverages to extract a bigger DFA, which is then used to identify erroneous strings.

Method. When the learned DFA $\hat{A}$ is not isomorphic to the target DFA $A^{\star}$, we construct the product automaton $B = \hat{A} \times A^{\star}$ where each state of B is a pair (p, q) with $p \in Q(\hat{A})$ and $q \in Q(A^{\star})$; on input symbol a, B transitions $\delta_B((p,q),a) = (\delta_{\hat{A}}(p,a), \delta_{A^{\star}}(q,a))$. The state (p,q) is accepting if and only if exactly one of p or q is accepting (XOR). The product DFA accepts the strings in the symmetric difference of the hypothesis and target DFA $L(B) = L(\hat{A}) \triangle L(A^{\star})$. We then enumerate erroneous strings by doing a BFS-like search within B to find accepting strings in nondecreasing length order.

Table 2: Examples of erroneous strings found via extracted DFAs. The $A^{\star}$ column within states denotes the number of states in the target DFA used to train the language model. The $\hat{A}$ column indicates the number of states in the extracted DFA. Ground truth labels are denoted by $y_{\star}$, and Teacher LM labels by y_T. Note: The models used as Teacher LM for Tomita-5, Dyck-$(2,2)$ and Dyck-$(3,3)$ for these results were imperfect and not the same models used for the experiments in Figure 2. See Sections 6 and G.2 for more details.

Language	**States** $\lvert A^{\star}\rvert$	$\lvert\hat{A}\rvert$	**Labels** $y_{\star}$	y_T	**Erroneous string** x
			1	0	0 0 1 0 0 0 0 0 0 0 0 0 0
Parity	2	26	0	1	0 0 1 0 0 0 0 0 0 0 0 0 0 1 0
			0	1	0 0 1 0 0 0 0 0 0 0 0 0 0 1 0 0
			0	1	( ) [ ] ( ) ( ) ( ) [ ] ( ) [ ]]
Dyck-(2,2)	8	189	0	1	[ ] [ ] ( ) ( ) ( ) [ ] ( ) [ ]]
			0	1	( ) [ ] ( ) ( ) ( ) [ ] ( ) [ ]] ( )
			0	1	{ { ( ) [ ] [ ] [ ] } ( ) { }
Dyck-(3,3)	41	87	0	1	{ { [ ] [ ] [ ] [ ] } ( ) { }
			0	1	{ { { } [ ] [ ] [ ] } ( ) { }
			0	1	0 1 1 0 0 1 1 0 0 1 0 1 0 1 0 1 1 0 1 0 1 0 1 0 0 1
Tomita-5	4	28	0	1	0 1 1 0 0 1 1 0 0 1 0 1 0 1 0 1 1 0 1 0 1 0 1 0 1 0
			0	1	0 1 1 0 0 1 1 0 0 1 0 1 0 1 1 0 1 0 1 0 1 0 1 0 0 1

Results. We observed erroneous strings for languages like Parity, Tomita-5, Dyck-$(2,2)$, and Dyck-$(3,3)$. Examples of some erroneous strings identified by the hypothesis DFA is provided in Table 2. Figure 6 and 7 show the DFAs extracted for Parity and Tomita-5, respectively. The DFAs for Dyck-$(2,2)$ and Dyck-$(3,3)$

Table 3: Usage of different types of NSP labels by the $\mathrm{L}^{\star}_{\mathrm{nsp}}$ algorithm on various tasks. Refinement indicates the number of times states were added through disagreements (number of times loop in Line 9 is executed or equivalently Lemma 5.1 is invoked. Mem fraction denotes the percentage of times prefix membership labels were used. B1 and B2 fractions denote how many continuation labels were used. See Sec. G.4 for more details.

Language	States	Prefix Memberships (%)	Cont. B1 (%)	Cont. B2 (%)	Refinements
Sample size: 10					
Dyck22	8.0 ± 0.0	0.0 ± 0.0	16.7 ± 0.0	$\mathbf{83.3 \pm 0.0}$	6.00 ± 0.00
Dyck24	21.0 ± 5.4	0.0 ± 0.0	5.9 ± 2.6	$\mathbf{94.1 \pm 2.6}$	19.00 ± 5.35
Dyck33	32.5 ± 7.0	0.0 ± 0.0	3.5 ± 1.2	$\mathbf{96.5 \pm 1.2}$	30.50 ± 7.01
Dyck43	37.4 ± 14.1	0.0 ± 0.0	3.8 ± 3.2	$\mathbf{96.2 \pm 3.2}$	35.40 ± 14.14
Parity	2.0 ± 0.0	$\mathbf{0.0 \pm 0.0}$	$\mathbf{0.0 \pm 0.0}$	$\mathbf{0.0 \pm 0.0}$	0.00 ± 0.00
Tomita 2	3.0 ± 0.0	0.0 ± 0.0	0.0 ± 0.0	$\mathbf{100.0 \pm 0.0}$	1.00 ± 0.00
Tomita 5	4.0 ± 0.0	$\mathbf{100.0 \pm 0.0}$	0.0 ± 0.0	0.0 ± 0.0	2.00 ± 0.00
Tomita 7	5.0 ± 0.0	0.0 ± 0.0	$\mathbf{100.0 \pm 0.0}$	0.0 ± 0.0	3.00 ± 0.00
Sample size: 100					
Dyck22	8.0 ± 0.0	0.0 ± 0.0	16.7 ± 0.0	$\mathbf{83.3 \pm 0.0}$	6.00 ± 0.00
Dyck24	32.0 ± 0.0	0.0 ± 0.0	3.3 ± 0.0	$\mathbf{96.7 \pm 0.0}$	30.00 ± 0.00
Dyck33	41.0 ± 0.0	0.0 ± 0.0	2.6 ± 0.0	$\mathbf{97.4 \pm 0.0}$	38.90 ± 0.32
Dyck43	85.6 ± 1.3	0.0 ± 0.0	1.2 ± 0.0	$\mathbf{98.8 \pm 0.0}$	83.60 ± 1.26
Parity	2.0 ± 0.0	$\mathbf{0.0 \pm 0.0}$	$\mathbf{0.0 \pm 0.0}$	$\mathbf{0.0 \pm 0.0}$	0.00 ± 0.00
Tomita 2	3.0 ± 0.0	0.0 ± 0.0	0.0 ± 0.0	$\mathbf{100.0 \pm 0.0}$	1.00 ± 0.00
Tomita 5	4.0 ± 0.0	$\mathbf{100.0 \pm 0.0}$	0.0 ± 0.0	0.0 ± 0.0	2.00 ± 0.00
Tomita 7	5.0 ± 0.0	0.0 ± 0.0	$\mathbf{100.0 \pm 0.0}$	0.0 ± 0.0	3.00 ± 0.00
Sample size: 1000					
Dyck22	8.0 ± 0.0	0.0 ± 0.0	16.7 ± 0.0	$\mathbf{83.3 \pm 0.0}$	6.00 ± 0.00
Dyck24	32.0 ± 0.0	0.0 ± 0.0	3.3 ± 0.0	$\mathbf{96.7 \pm 0.0}$	30.00 ± 0.00
Dyck33	41.0 ± 0.0	0.0 ± 0.0	2.6 ± 0.0	$\mathbf{97.4 \pm 0.0}$	39.00 ± 0.00
Dyck43	86.0 ± 0.0	0.0 ± 0.0	1.2 ± 0.0	$\mathbf{98.8 \pm 0.0}$	84.00 ± 0.00
Parity	18.3 ± 15.7	$\mathbf{70.0 \pm 48.3}$	0.0 ± 0.0	0.0 ± 0.0	11.80 ± 11.72
Tomita 2	3.0 ± 0.0	0.0 ± 0.0	0.0 ± 0.0	$\mathbf{100.0 \pm 0.0}$	1.00 ± 0.00
Tomita 5	4.0 ± 0.0	$\mathbf{100.0 \pm 0.0}$	0.0 ± 0.0	0.0 ± 0.0	2.00 ± 0.00
Tomita 7	5.0 ± 0.0	0.0 ± 0.0	$\mathbf{100.0 \pm 0.0}$	0.0 ± 0.0	3.00 ± 0.00

are too large to be visually interpretable. Constructing the product DFA is efficient and identifying several erroneous examples takes only a few seconds. There is no natural distribution over the symmetric difference language and further it can even be finite in some cases which makes it difficult to systematically compute the accuracy of predicting erroneous examples using the extracted DFA. The closest signal we have is the NSP accuracy for the extracted DFAs which is near perfect.

Fortunately, identifying strings in the symmetric difference language of $\hat{A}$ and $A^{\star}$ is quite efficient which can allow one to find numerous erroneous examples (if they exist). For instance, with 1k strings generated from Transformer trained on Parity, the $\mathrm{L}^{\star}_{\mathrm{nsp}}$ algorithm extracted a DFA with 26 states within 10 seconds, and using the extracted DFA, we identified 1k strings in the symmetric difference language $L(\hat{A}) \triangle L(A^{\star})$ in 16 seconds. Out of the 1000 strings identified by $\hat{A}$, 987 of them were erroneous: $A^{\star}(x) \neq \mathrm{MQ}(x)$ where $\mathrm{MQ}(x)$ denotes whether the string was in the support of the teacher language model and $A^{\star}(x)$ indicates whether the string was in the target regular language. Thus, such an approach can sometimes be far more efficient than finding erroneous strings by repeatedly sampling from a language model and testing whether they are correct or not.

For all languages except Parity, the language model became more robust when we retrained them for longer steps. The curves for Tomita-5, and the two Dyck languages in Fig. 2 are with retrained and more accurate Transformer models. We suspect that for the lengths considered in this paper, retraining a larger Transformer on Parity for longer might make it more robust, but we keep the imperfect model to illustrate the differences in Fig. 2.

G.3 Practical Notes on the algorithm

As mentioned in Sec. 7, if the DFA representing the support of the language model has a large number of states, then the extraction algorithm can be extremely slow. The key bottleneck for $\mathrm{L}^\star_{\mathrm{nsp}}$ is the same as $\mathrm{L}^\star$, which is the closure step (Line 22 in Alg. 1). Even though it is polynomial, the time complexity $O(|Q||T||\Sigma|)$ blows up when both $|Q|$ and $|T|$ are in the order of thousands, since the process is sequential. We observe that when the models are partially or poorly trained, then the number of states blows up, and the algorithm slows down significantly, failing to terminate even after a day.

The other step where the $\mathrm{L}^\star_{\mathrm{nsp}}$ algorithm might fail is if the assumptions about the learning problem are violated, in which case the use of generative queries to find accepting suffixes (Line 18 in Alg. 1) may not terminate. If the support language is not regular, then even though a continuation is permissible according to min-p/top-p sampling, the language model may still not terminate. However, we did not observe any instance of this problem in all our experiments. We suspect that since the language models are typically trained to predict [EOS] after a certain steps, they always terminate (the EOS token becomes permissible) after a certain number of inference steps.

G.4 Ablation: Usage of Continuation Labels

When we apply the $\mathrm{L}^\star_{\mathrm{nsp}}$ algorithm on positive examples, information about refinements or new states is provided by two types of labels: (i) prefix membership labels, and (ii) continuation labels. Within continuation labels, there are two cases as described in Lemma. 5.1. Whenever the algorithm finds one of the three types of disagreements in the NSP labels between the hypothesis DFA and the examples in its set, it refines the DFA and adds one more state to its hypothesis.

Results. We run the $\mathrm{L}^\star_{\mathrm{nsp}}$ algorithm on 8 representative languages and track the usage of the type of disagreement used to update its hypothesis. Table 3 depicts the usage of different types of disagreements on three different sample sizes averaged across 10 runs. The prefix membership column indicates the percentage of times the prefix membership labels were used. The Cont. B1 column represents the cases where the hypothesis predicted that a certain continuation is permitted, but the continuation label indicated that no such continuation is allowed in the target DFA. The Cont. B2 column represents the cases where the hypothesis predicts that continuation is forbidden, but the true labels indicate otherwise. This is the case where the generative query oracle is invoked to generate accepting suffixes. See Sec. 5 for the details of the algorithm.

The results indicate that continuation labels are heavily used for all Dyck languages. Such languages also contain several transitions with dead states, and the results indicate that the algorithm is able to leverage continuation labels to identify new states. On parity and Tomita-5, the algorithm relies only on the prefix membership labels. This is natural since the DFAs for those languages do not have any dead states, and hence the continuation labels are uninformative. From positive examples, the algorithm can obtain negative information from the prefix membership labels for such languages. Both Tomita-2 and Tomita-7 have a transition to a dead state. Since these are small DFAs, the algorithm converges to the target DFA with only a few refinements.