Automata for Hyperlanguages

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Abstract

Hyperproperties lift conventional trace properties from a set of execution traces to a set of sets of execution traces. Hyperproperties have been shown to be a powerful formalism for expressing and reasoning about information-flow security policies and important properties of cyber-physical systems such as sensitivity and robustness, as well as consistency conditions in distributed computing such as linearizability. Although there is an extensive body of work on automata-based representation of trace properties, we currently lack such characterization for hyperproperties.

We introduce hyperautomata for hyperlanguages, which are languages over sets of words. Essentially, hyperautomata allow running multiple quantified words over an automaton. We propose a specific type of hyperautomata called nondeterministic finite hyperautomata (NFH), which accept regular hyperlanguages. We demonstrate the ability of regular hyperlanguages to express hyperproperties for finite traces. We then explore the fundamental properties of NFH and show their closure under the Boolean operations. We show that while nonemptiness is undecidable in general, it is decidable for several fragments of NFH. We further show the decidability of the membership problem for finite sets and regular languages for NFH, as well as the containment problem for several fragments of NFH. Finally, we introduce learning algorithms based on Angluin’s $L^*$ algorithm for the fragments NFH in which the quantification is either strictly universal or strictly existential.

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1 Introduction

Hyperproperties [7] generalize the traditional trace properties [1] to system properties, i.e., a set of sets of traces. Put another way, a hyperproperty prescribes how the system should behave in its entirety and not just based on its individual executions. Hyperproperties have been shown to be a powerful tool for expressing and reasoning about information-flow security policies [7] and important properties of cyber-physical systems [16] such as sensitivity and robustness, as well as consistency conditions in distributed computing such as linearizability [4].

Automata theory has been in the forefront of developing techniques for specification and verification of computing systems. For instance, in the automata-theoretic approach to verification [14, 15], the model-checking problem is reduced to checking the nonemptiness of the product automaton of the model and the complement of the specification. In the industry and other disciplines (e.g., control theory), automata are an appealing choice for modeling the behavior of a system. Unfortunately, we currently lack a deep understanding about the relation between hyperproperties and automata theory. To our knowledge, work in this area is limited to [8], in which the authors develop an automata representation for the class of regular k-safety hyperproperties. These are hyperproperties where execution traces are only universally quantified and their behaviors are non-refutable. They introduce the notion of a k bad-prefix automaton – a finite-word automaton that recognizes sets of k bad prefixes as finite words. Based on this representation, they present a learning algorithm for k-safety hyperproperties. In [10], the authors offer a model-checking algorithm for hyperCTL* [6], which constructs an alternating Büchi automaton that has both the formula and the Kripke structure “built-in”. These approaches translate a hyperproperty-related problem to word automata.

We generalize the idea in [8] to a broader view of an automata-based representation of hyperproperties, and introduce hyperautomata for hyperlanguages, which are languages whose elements are sets of finite words, which we call hyperwords. In this paper, we propose nondeterministic finite-word hyperautomata (NFH). An NFH runs on hyperwords that contain finite words, by using quantified word variables that range over the words in a hyperword, and a nondeterministic finite-word automaton (NFA) that runs on the set of words that are assigned to the variables. We demonstrate the idea with two examples.

► Example 1. Consider the NFH A1 in Figure 1 (left), whose alphabet is Σ = {a, b}, over two word variables x1 and x2. The NFH A1 contains an underlying standard NFA, whose alphabet comprises pairs over Σ, i.e., elements of Σ2, in which the first letter represents the letters of the word assigned to x1, and dually for the second letter and x2. The underlying NFA of A1 requires that (1) these two words agree on their a (and, consequently, on their b) positions, and (2) once one of the words has ended (denoted by #), the other must only contain b letters. Since the quantification condition of A1 is ∀x1 ∃x2, in a hyperword S that is accepted by A1, every two words agree on their a positions. As a result, all the words in S must agree on their a positions. The hyperlanguage of A1 is then all hyperwords in which all words agree on their a positions.

► Example 2. Next, consider the NFH A2 in Figure 1 (right), over the alphabet Σ = {a}, and two word variables x1 and x2. The underlying NFA of A2 accepts the two words assigned to x1 and x2 iff the word assigned to x2 is longer than the word assigned to x1. Since the quantification condition of A2 is ∀x1 ∃x2, we have that A2 requires that for every word in a hyperword S accepted by A2, there exists a longer word in S. This holds iff S contains infinitely many words. Therefore, the hyperlanguage of A2 is the set of all infinite hyperwords over {a}.

We call the hyperlanguages accepted by NFH regular hyperlanguages. A regular hyperlanguage L can also be expressed by the regular expression for the language of the underlying NFA of an NFH A for L, augmented with the quantification condition of A. We call such an expression a hyperregular
expression (HRE). We demonstrate the ability of HREs to express important information-flow security policies such as different variations of noninterference [11] and observational determinism [17].

We proceed to conduct a comprehensive study of properties of NFH (see Table 1). In particular, we show that NFH are closed under union, intersection, and complementation. We also prove that the nonemptiness problem is in general undecidable for NFH. However, for the alternation-free fragments (which only allow one type of quantifier), as well as for the ∃∀ fragment (in which the quantification condition is limited to a sequence of ∃ quantifiers followed by a sequence of ∀ quantifiers), nonemptiness is decidable. These results are in line with the results on satisfiability of HyperLTL [9]. We also study the membership and inclusion problems. These results are aligned with the complexity of HyperLTL model checking for tree-shaped and general Kripke structures [3]. This shows that, surprisingly, the complexity results in [9, 3] mainly stem from the nature of quantification over finite words and depend on neither the full power of the temporal operators nor the infinite nature of HyperLTL semantics.

Finally, we introduce learning algorithms for the alternation-free fragments of NFH. Our algorithms are based on Angluin’s L* algorithm [2] for regular languages, and are inspired by [8], where the authors describe a learning algorithm that is tailored to learn a k-bad prefix NFA for a k-safety formula. In fact, the algorithm there can be viewed as a special case of learning a hyperlanguage in the ∃-fragment of NFH.

In a learning algorithm, a learner aims to construct an automaton for an unknown target language $L$, by means of querying a teacher, who knows $L$. The learner asks two types of queries: membership queries ("is the word $w$ in $L$?") and equivalence queries ("is $A$ an automaton for $L$?"). In case of a failed equivalence query, the teacher returns a counterexample word on which $A$ and $L$ differ. The learning algorithm describes how the learner uses the answers it gets from the teacher to construct its candidate automaton.

In the case of NFH, the membership queries, as well as the counterexamples, are hyperwords. The number of variables is unknown in advance, and is also part of the learning goal. We first define canonical forms for the alternation-free fragments of NFH, which is essential for this type of learning algorithm. Then, we proceed to describe the learning algorithms for both fragments.

Organization. The rest of the paper is organized as follows. Preliminary concepts are presented in Section 2. We introduce the notion of NFH and HRE in Sections 3 and 4, while their properties are studied in Section 5. We propose our learning algorithm in Section 6. Finally, we make concluding remarks and discuss future work in Section 7. Detailed proofs appear in the appendix.

2 Preliminaries

An alphabet is a nonempty finite set $Σ$ of letters. A word over $Σ$ is a finite sequence of letters from $Σ$. The empty word is denoted by $ϵ$, and the set of all finite words is denoted by $Σ^*$. A language is a subset of $Σ^*$.

Definition 3. A nondeterministic finite-word automaton (NFA) is a tuple $A = (Σ, Q, Q_0, δ, F)$, where $Σ$ is an alphabet, $Q$ is a nonempty finite set of states, $Q_0 ⊆ Q$ is
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| Property          | Result                                      |
|-------------------|---------------------------------------------|
| Closure           | Complementation, Union, Intersection (Theorem 8) |
| Nonemptiness      | $\exists \exists^*/\forall^*$ Undecidable (Theorem 9) |
|                   | $\exists^*/\forall^*$ NL-complete (Theorem 10) |
|                   | $\exists^*/\forall^*$ PSPACE-complete (Theorem 11) |
| Finite membership | NFH PSPACE (Theorem 12)                      |
|                   | $O(\log(k)) \forall$ NP-complete (Theorem 12) |
| Regular membership| Decidable (Theorem 13)                      |
| Containment       | $\exists^*/\forall^*/\exists^*/\forall^* \subseteq \exists^*/\forall^*$ PSPACE-complete (Theorem 14) |

Table 1: Summary of results on properties of NHF.

A set of initial states, $F \subseteq Q$ is a set of accepting states, and $\delta \subseteq Q \times \Sigma \times Q$ is a transition relation.

Given a word $w = \sigma_1 \sigma_2 \ldots \sigma_n$ over $\Sigma$, a run of $A$ on $w$ is a sequence of states $(q_0, q_1, \ldots q_n)$, such that $q_0 \in Q_0$, and for every $0 < i \leq n$, it holds that $(q_{i-1}, \sigma_i, q_i) \in \delta$. The run is accepting if $q_n \in F$. We say that $A$ accepts $w$ if there exists an accepting run of $A$ on $w$. The language of $A$, denoted by $L(A)$, is the set of all finite words that $A$ accepts. A language $L$ is called regular if there exists an NFA such that $L(A) = L$.

An NFA $A$ is called deterministic (DFA), if for every $q \in Q$ and $\sigma \in \Sigma$, there exists exactly one $q'$ for which $(q, \sigma, q') \in \delta$, i.e., $\delta$ is a transition function. It is well-known that every NFA has an equivalent DFA.

3  Hyperautomata

Before defining hyperautomata, we explain the idea behind them. We first define hyperwords and hyperlanguages.

Definition 4. A hyperword over $\Sigma$ is a set of words over $\Sigma$ and a hyperlanguage is a set of hyperwords.

A hyperautomaton $A$ uses a set of word variables $X = \{x_1, x_2, \ldots, x_k\}$. When running on a hyperword $S$, these variables are assigned words from $S$. We represent an assignment $v : X \rightarrow S$ as the $k$-tuple $(v(x_1), v(x_2), \ldots, v(x_k))$. Notice that the variables themselves do not appear in this representation of $v$, and are manifested in the order of the words in the $k$-tuple: the $i$'th word is the one assigned to $x_i$. This allows a cleaner representation with less notations.

The hyperautomaton $A$ consists of a quantification condition $\alpha$ over $X$, and an underlying word automaton $\hat{A}$, which runs on words that represent assignments to $X$ (we explain how we represent assignments as words later on). The condition $\alpha$ defines the assignments that $\hat{A}$ should accept. For example, $\alpha = \exists x_1 \forall x_2$ requires that there exists a word $w_1 \in S$ (assigned to $x_1$), such that for every word $w_2 \in S$ (assigned to $x_2$), the word that represents $(w_1, w_2)$ is accepted by $\hat{A}$. The hyperword $S$ is accepted by $A$ iff $S$ meets these conditions.

We now elaborate on how we represent an assignment $v : X \rightarrow S$ as a word. We encode the tuple $(v(x_1), v(x_2), \ldots, v(x_k))$ by a word $w$ whose letters are $k$-tuples in $\Sigma^k$, where the $i$'th letter of $w$ represents the $k$ $i$'th letters of the words $v(x_1), \ldots, v(x_k)$ (in case that the words are not of equal length, we “pad” the end of the word with # signs). For example, the assignment $v(x_1) = aa, v(x_2) = abb$, represented by the tuple $(aa, abb)$, is encoded by the word $(a, a)(a, b)(\# , b)$. We later refer to $w$ as the zipping of $v$. Once again, notice that due to the indexing of the word variables, the variables do not explicitly appear in $w$. 

a set of initial states, $F \subseteq Q$ is a set of accepting states, and $\delta \subseteq Q \times \Sigma \times Q$ is a transition relation.
We now turn to formally define hyperautomata.

### 3.1 Nondeterministic Finite-Word Hyperautomata

We begin with some terms and notations.

Let \( s = (w_1, w_2, \ldots, w_k) \) be a tuple of finite words over \( \Sigma \). We denote the length of the longest word in \( s \) by \( |s| \). We represent \( s \) by a word over \( (\Sigma \cup \{\#\})^k \) of length \( |s| \), which is formed by a function \( \text{zip}(s) \) that “zips” the words in \( s \) together: the \( i \)’th letter in \( \text{zip}(s) \) represents the \( i \)’th letters in \( w_1, w_2, \ldots, w_k \), and \# is used to pad the words that have ended. For example,

\[
\text{zip}(aab, bc, abdd) = (a, b, a)(a, c, b)(b, \#, d)(\#, \#, \#),
\]

Formally, we have \( \text{zip}(s) = s_1s_2 \cdots s_{|s|} \), where \( s_i[j] = w_j \), if \( j \leq |w_j| \), and \( s_i[j] = \# \), otherwise.

Given a zipped word \( s \), we denote the word formed by the letters in the \( i \)’th positions in \( s \) by \( s[i] \). That is, \( s[i] \) is the word \( \sigma_1\sigma_2 \cdots \sigma_n \), formed by defining \( \sigma_j = s_j[i] \), for \( s_j[i] \in \Sigma \). Notice that \( \text{zip}(s) \) is reversible, and we can define an unzip function as \( \text{unzip}(s) = (s[1], s[2], \ldots, s[k]) \). We sometimes abuse the notation, and use \( \text{unzip}(s) \) to denote \( \{s[1], s[2], \ldots, s[k]\} \), and \( \text{zip}(S) \) to denote the zipping of the words in a finite hyperword \( S \) in some arbitrary order.

> **Definition 5.** A nondeterministic finite-word hyperautomaton (NFH) is a tuple \( A = (\Sigma, X, Q_0, F, \delta, \alpha) \), where \( \Sigma, Q, Q_0, \) and \( F \) are as in Definition 3, \( X = \{x_1, \ldots, x_k\} \) is a finite set of word variables, \( \delta \subseteq Q \times (\Sigma \cup \{\#\})^k \times Q \) is a transition relation, and \( \alpha = Q_1 x_1 Q_2 x_2 \cdots Q_n x_k \) is a quantification condition, where \( Q_i \in \{\forall, \exists\} \) for every \( 1 \leq i \leq k \).

In Definition 5, the tuple \((\Sigma \cup \{\#\})^k, Q, Q_0, \delta, F\) forms an underlying NFA of \( A \), which we denote by \( \hat{A} \). We denote the alphabet of \( \hat{A} \) by \( \Sigma \).

Let \( S \) be a hyperword and let \( v : X \rightarrow S \) be an assignment of the word variables of \( A \) to words in \( S \). We denote by \( v[x \rightarrow w] \) the assignment obtained from \( v \) by assigning the word \( w \) to \( x \) in \( X \). We represent \( v \) by the word \( \text{zip}(v) = \text{zip}(v(x_1), \ldots, v(x_k)) \). We now define the acceptance condition of a hyperword \( S \) by an NFH \( A \). We first define the satisfaction relation \( \models \) for \( S, A \), a quantification condition \( \alpha \), and an assignment \( v : X \rightarrow S \), as follows.

- For \( \alpha = \epsilon \), we denote \( S \models_{v} (\alpha, A) \) if \( \hat{A} \) accepts \( \text{zip}(v) \).
- For \( \alpha = \exists x \alpha' \), we denote \( S \models_{v} (\alpha, A) \) if there exists \( w \in S \) such that \( S \models_{v[x \rightarrow w]} (\alpha', A) \).
- For \( \alpha = \forall x \alpha' \), we denote \( S \models_{v} (\alpha, A) \) if for every \( w \in S \), it holds that \( S \models_{v[x \rightarrow w]} (\alpha', A) \).

Since the quantification condition of \( A \) includes all of \( X \), the satisfaction is independent of the assignment \( v \), and we denote \( S \models A \), in which case, we say that \( A \) accepts \( S \).

> **Definition 6.** Let \( A \) be an NFH. The hyperlanguage of \( A \), denoted \( \mathcal{L}(A) \), is the set of all hyperwords that \( A \) accepts.

We call a hyperlanguage \( \mathcal{L} \) a regular hyperlanguage if there exists an NFH \( A \) such that \( \mathcal{L}(A) = \mathcal{L} \).

> **Example 7.** Consider the NFH \( A_3 \) in Figure 2, over the alphabet \( \Sigma = \{a, b\} \) and two word variables \( x_1 \) and \( x_2 \). From the initial state, two words lead to the left component in \( A_3 \) iff in every position, if the word assigned to \( x_2 \) has an \( a \), the word assigned to \( x_1 \) has an \( a \). In the right component, the situation is dual – in every position, if the word assigned to \( x_1 \) has an \( a \), the word assigned to \( x_2 \) has an \( a \). Since the quantification condition of \( A_3 \) is \( \forall x_1 \forall x_2 \), in a hyperword \( S \) accepted by \( A_3 \), in every two words in \( S \), the set of \( a \) positions of one is a subset of the \( a \) positions of the other. Therefore, \( \mathcal{L}(A_3) \) includes all hyperwords in which there is a full ordering on the \( a \) positions.

\(^2\) In case that \( \alpha \) begins with \( \forall \), satisfaction holds vacuously with an empty hyperword. We restrict the discussion to nonempty hyperwords.
We now show the application of HREs in specifying well-known information-flow security policies.

3.2 Additional Terms and Notations

We present several more terms and notations which we use throughout the following sections. We say that a word \( w \) over \( (\Sigma \cup \#)^k \) is legal if \( w = \text{zip}(u_1, \ldots, u_k) \) for some \( u_1, u_2, \ldots, u_k \in \Sigma^* \). Note that \( w \) is legal if and only if there is no \( w[i] \) in which there is an occurrence of \( \# \) followed by some letter \( \sigma \in \Sigma \).

Consider two letter tuples \( \sigma_1 = (t_1, \ldots, t_k) \) and \( \sigma_2 = (s_1, \ldots, s_k) \). We denote by \( \sigma_1 + \sigma_2 \) the tuple \( (t_1, \ldots, t_k, s_1, \ldots, s_k) \). We extend the notion to zipped words. Let \( w_1 = \text{zip}(u_1, \ldots, u_k) \) and \( w_2 = \text{zip}(v_1, \ldots, v_k) \). We denote by \( w_1 + w_2 \) the word \( \text{zip}(u_1, \ldots, u_k, v_1, \ldots, v_k) \).

Consider a tuple \( t = (t_1, t_2, \ldots, t_k) \) of items. A sequence of \( t \) is a tuple \( (t'_1, t'_2, \ldots, t'_k) \), where \( t'_i \in \{ t_1, \ldots, t_k \} \) for every \( 1 \leq i \leq k \). A permutation of \( t \) is a reordering of the elements of \( t \). We extend these notions to zipped words, to assignments, and to hyperwords, as follows. Let \( \zeta = (i_1, i_2, \ldots, i_k) \) be a sequence (permutation) of \( (1, 2, \ldots, k) \).

- Let \( \bfw = \text{zip}(w_1, \ldots, w_k) \) be a word over \( k \)-tuples. The word \( \bfw_\zeta \), defined as \( \text{zip}(w_{i_1}, w_{i_2}, \ldots, w_{i_k}) \) is a sequence (permutation) of \( \bfw \).
- Let \( v \) be an assignment from a set of variables \( \{ x_1, x_2, \ldots, x_k \} \) to a hyperword \( S \). The assignment \( v_\zeta \), defined as \( v_\zeta(x_{j}) = v(x_{i_j}) \) for every \( 1 \leq i_j, j \leq k \), is a sequence (permutation) of \( v \).
- Let \( S \) be a hyperword. The tuple \( \bfw = (w_1, \ldots, w_k) \), where \( w_i \in S \), is a sequence of \( S \). if \( \{ w_1, \ldots, w_k \} = S \), then \( \bfw \) is a permutation of \( S \).

4 Hyperregular Expressions and Application in Security

Given an NFH \( \mathcal{A} \), the language of its underlying NFA \( \hat{\mathcal{A}} \) can be expressed as a regular expression \( r \). Augmenting \( r \) with the quantification condition \( \alpha \) of \( \mathcal{A} \) constitutes a hyperregular expression (HRE) \( \alpha r \). For example, consider the NFH \( \mathcal{A}_1 \) in Figure 1. The HRE of \( \mathcal{A}_1 \) is:

\[
\forall x_1 \forall x_2 \left( (a, a) \mid (b, b) \right)^* \left( \left( \#, b \right)^* \mid (b, \#)^* \right)^*
\]

We now show the application of HREs in specifying well-known information-flow security policies. Noninterference [11] requires that commands issued by users holding high clearances be removable without affecting observations of users holding low clearances:

\[
\varphi_{ni} = \forall x_1 \exists x_2 (l, l)^*
\]

where \( l \) denotes a low state and \( l \lambda \) denotes a low state where all high commands are replaced by a dummy value \( \lambda \).
Observational determinism [17] requires that if two executions of a system start with low-security-equivalent events, then these executions should remain low equivalent:

$$\varphi_{od} = \forall x_1 \forall x_2 \exists l, l^+ \left( (l, l) \in (\Sigma, \Sigma)^* \right) \left( (l, l) (\$, \$) \in (\Sigma, \Sigma)^* \right)$$

where \( l \) denotes a low event, \( \bar{l} \in \Sigma \setminus \{l\} \), and \( \$ \in \Sigma \). We note that similar policies such as Boudol and Castellani’s noninterference [5] can be formulated in the same fashion.

Generalized noninterference (GNI) [12] allows nondeterminism in the low-observable behavior, but requires that low-security outputs may not be altered by the injection of high-security inputs:

$$\varphi_{gni} = \forall x_1 \forall x_2 \exists l_1, l_2 \left( (l_1, l_2) \in (\Sigma, \Sigma)^* \right) \left( (l_1, l_2) (\$, \$) \in (\Sigma, \Sigma)^* \right)$$

where \( h \) denotes the high-security input, \( l \) denotes the low-security output, \( \bar{l} \in \Sigma \setminus \{l\} \), and \( \bar{h} \in \Sigma \setminus \{h\} \).

Declassification [13] relaxes noninterference by allowing leaking information when necessary. Some programs need to reveal secret information to fulfill functional requirements. For example, a password checker must reveal whether the entered password is correct or not:

$$\varphi_{dc} = \forall x_1 \forall x_2 \exists l, l^+ \left( (l, l) \in (\Sigma, \Sigma)^* \right) \left( (l, l) (\$, \$) \in (\Sigma, \Sigma)^* \right)$$

where \( l_i \) denotes low-input state, \( pw \) denotes that the password is correct, and \( lo \) denotes low-output states. We note that for brevity, in the above formula, we do not include behaviors where the first two events are not low or in the second event, the password is not valid.

Termination-sensitive noninterference requires that for two executions that start from low-observable states, information leaks are not permitted by the termination behavior of the program:

$$\varphi_{tsni} = \forall x_1 \forall x_2 \exists l, l^+ \left( (l, l) \in (\Sigma, \Sigma)^* \right) \left( (l, l) (\$, \$) \in (\Sigma, \Sigma)^* \right)$$

where \( l \) denotes a low state and \( \$ \in \Sigma \).

5 Properties of Regular Hyperlanguages

In this section, we consider the basic operations and decision problems for the various fragments of NFH. We mostly provide proof sketches, and the complete details appear in the appendix. Throughout this section, \( \mathcal{A} \) is an NFH \( \langle \Sigma, X, Q, Q_0, \delta, F, \alpha \rangle \), where \( X = \{x_1, \ldots, x_k\} \).

We first show that NFH are closed under all the Boolean operations.

Theorem 8. NFH are closed under union, intersection, and complementation.

Proof Sketch. Complementing \( \mathcal{A} \) amounts to dualizing its quantification condition (replacing every \( \exists \) with \( \forall \) and vice versa), and complementing \( \mathcal{A} \) via the standard construction for NFA.

Now, let \( \mathcal{A}_1 \) and \( \mathcal{A}_2 \) be two NFH. The NFH \( \mathcal{A}_\cap \) for \( \Sigma(\mathcal{A}_1) \cap \Sigma(\mathcal{A}_2) \) is based on the product construction of \( \mathcal{A}_1 \) and \( \mathcal{A}_2 \). The quantification condition of \( \mathcal{A}_\cap \) is \( \alpha_1 \cdot \alpha_2 \). The underlying automaton \( \hat{\mathcal{A}}_\cap \) advances simultaneously on both \( \mathcal{A}_1 \) and \( \mathcal{A}_2 \); when \( \hat{\mathcal{A}}_1 \) and \( \hat{\mathcal{A}}_2 \) run on zipped hyperwords \( w_1 \) and \( w_2 \), respectively, \( \hat{\mathcal{A}}_\cap \) runs on \( w_1 + w_2 \), and accepts only if both \( \hat{\mathcal{A}}_1 \) and \( \hat{\mathcal{A}}_2 \) accept.

Similarly, the NFH \( \mathcal{A}_\cup \) for \( \Sigma(\mathcal{A}_1) \cup \Sigma(\mathcal{A}_2) \) is based on the union construction of \( \hat{\mathcal{A}}_1 \) and \( \hat{\mathcal{A}}_2 \). The quantification condition of \( \mathcal{A}_\cup \) is again \( \alpha_1 \cdot \alpha_2 \). The underlying automaton \( \hat{\mathcal{A}}_\cup \) advances either on \( \mathcal{A}_1 \) or \( \mathcal{A}_2 \). For every word \( w \) read by \( \hat{\mathcal{A}}_1 \), the NFH \( \hat{\mathcal{A}}_\cup \) reads \( w + w' \), for every \( w' \in \Sigma_2^* \), and dually, for every word \( w \) read by \( \hat{\mathcal{A}}_2 \), the NFH \( \hat{\mathcal{A}}_\cup \) reads \( w' + w \), for every \( w' \in \Sigma_1^* \).
We now turn to study various decision problems for NFH. We begin with the nonemptiness problem: given an NFH $A$, is $\Sigma(A) = \emptyset$? We show that while the problem is in general undecidable for NFH, it is decidable for the fragments that we consider.

**Theorem 9.** The nonemptiness problem for NFH is undecidable.

The proof of Theorem 9 mimics the ideas in [9], which uses a reduction from the Post correspondence problem (PCP) to prove the undecidability of HyperLTL satisifiability.

For the alternation-free fragments, we can show that a simple reachability test on their underlying automata suffices to verify nonemptiness. Hence, we have the following.

**Theorem 10.** The nonemptiness problem for NFH$_3$ and NFH$_\forall$ is $NL$-complete.

The nonemptiness of NFH$_{3\forall}$ is harder, and reachability does not suffice. However, we show that the problem is decidable.

**Theorem 11.** The nonemptiness problem for NFH$_{2\forall}$ is $PSPACE$-complete.

**Proof Sketch.** We can show that an NFH$_{2\forall}A$ is nonempty iff it accepts a hyperword $S$ of size that is bounded by the number $m$ of $\exists$ quantifiers in $A$. We can then construct an NFA $A$ whose language is nonempty iff it accepts $\text{zip}(S)$ for such a hyperword $S$. The size of $A$ is $O(|\delta|^{m^{k-m}})$. Unless $A$ only accepts hyperwords of size 1, which can be easily checked, $|\delta|$ must be exponential in the number $k - m$ of $\forall$ quantifiers, to account for all the assignments to the variables under $\forall$, and so overall $|A|$ is of size $O(|A|^k)$. The problem can then be decided in $PSPACE$ by traversing $A$ on-the-fly. We show that a similar result holds for the case that $k - m$ is fixed.

We use a reduction from the unary version of the tiling problem to prove $PSPACE$ lower bounds for both the general case and for the case of a fixed number of $\forall$ quantifiers.

We turn to study the membership problem for NFH: given an NFH $A$ and a hyperword $S$, is $S \in \Sigma(A)$? When $S$ is finite, the set of possible assignments from $X$ to $S$ is finite, and so the problem is decidable. We call this case the finite membership problem.

**Theorem 12.** The finite membership problem for NFH is in $PSPACE$. The finite membership problem for NFH with $O(\log(k))$ $\forall$ quantifiers is $NP$-complete.

**Proof Sketch.** We can decide the membership of a hyperword $S$ in $\Sigma(A)$ by iterating over all relevant assignments from $X$ to $S$, and for every such assignment $v$, checking on-the-fly whether $\text{zip}(v)$ is accepted by $A$. This algorithm uses space of size that is polynomial in $k$ and logarithmic in $|A|$ and in $|S|$. When the number of $\forall$ quantifiers in $A$ is $|O(\log(k))|$, we can iterate over all assignments to the $\forall$ variables in polynomial time, while guessing assignments to the variables under $\exists$. Thus, membership in this case is in $NP$.

We use a reduction from the Hamiltonian cycle problem to prove $NP$-hardness for this case. Given a graph $G = (\{v_1, \ldots, v_n\}, E)$, we construct a hyperword $S$ with $n$ different words of length $n$ over $\{0, 1\}$, each of which contains a single 1. We also construct an NFH$_3A$ over $\{0, 1\}$ with $n$ variables, a graph construction similar to that of $G$, and a single accepting and initial state $v_1$. From vertex $v_i$ there are transitions to all its neighbors, labeled by the letter $(0)^{i-1} + (1) + (0)^{n-i}$. Thus, $A$ accepts $S$ if there exists an assignment $f : X \rightarrow S$ such that $\text{zip}(f) \in \Sigma(A)$. Such an assignment $f$ describes a cycle in $G$, where $f(x_i) = w_j$ matches traversing $v_i$ in the $j$'th step. The words in $S$ ensure a single visit in every state, and their length ensures a cycle of length $n$.

**Note:** for every hyperword of size at least 2, the number of transitions in $\delta$ must be exponential in the number $k'$ of $\forall$ quantifiers, to account for all the different assignments to these variables. Thus, if $k = O(k')$, an algorithm that uses a space of size $k$ is in fact logarithmic in the size of $A$. ☐
When $S$ is infinite, it may still be finitely represented. We now address the problem of deciding whether a regular language $L$ (given as an NFA) is accepted by an NFH. We call this the regular membership problem for NFH. We show that this problem is decidable for the entire class of NFH.

Theorem 13. The regular membership problem for NFH is decidable.

Proof Sketch. Let $A$ be an NFA, and let $\mathcal{A}$ be an NFH, both over $\Sigma$. We describe a recursive procedure for deciding whether $L(A) \in L(\mathcal{A})$.

For the base case of $k = 1$, if $\alpha = \exists x_1$, then $L(A) \in L(\mathcal{A})$ iff $L(A) \cap L(\overline{A}) \neq \emptyset$. Otherwise, if $\alpha = \forall x_1$, then $L(A) \in L(\mathcal{A})$ iff $L(A) \notin L(\overline{A})$, where $\overline{A}$ is the NFH for $\overline{\Sigma(A)}$. The quantification condition for $\overline{A}$ is $\exists x_1$, which conforms to the previous case.

For $k > 1$, we construct a sequence of NFH $A_1, A_2, \ldots, A_k$. If $\alpha$ starts with $\exists$, then we set $A_1 = A$. Otherwise, we set $A_1 = \overline{A}$. Given $A_i$ with a quantification condition $\alpha_i$, we construct $A_{i+1}$ as follows. If $\alpha_i$ starts with $\exists$, then the set of variables of $A_{i+1}$ is $\{x_{i+1}, \ldots, x_k\}$, and the quantification condition $\alpha_{i+1} = Q_{i+1} x_{i+1} \cdots Q_k x_k$, where $\alpha_{i+1} = \exists Q_i x_i Q_{i+1} \cdots Q_k x_k$. The NFH $A_{i+1}$ is roughly constructed as the intersection between $A$ and $\overline{A_i}$, based on the first position in every $(k-i)$-tuple letter in $S_i$. Then, $\overline{A_{i+1}}$ accepts a word $(u_1, \ldots, u_{k-1})$ iff there exists a word $u \in L(A_i)$ such that $\overline{A_i}$ accepts $(u, u_1, \ldots, u_{k-1})$. Notice that this exactly conforms to the $\exists$ condition. Therefore, if $Q_i = \exists$, then $L(A) \in L(A_i)$ iff $L(A) \in L(\overline{A_{i+1}})$.

If $Q_i = \forall$, then $L(A) \in L(A_i)$ iff $L(A) \notin L(\overline{A_i})$. The quantification condition for $\overline{A_i}$ begins with $\exists x_i$. We then construct $A_{i+1}$ w.r.t. $\overline{A_i}$ as described above, and check for non-membership.

Every $\forall$ quantifier requires complementation, which is exponential in $|Q|$. Therefore, in the worst case, the complexity of this algorithm is $O(2^{2^{|Q||A|}})$, where the tower is of height $k$. If the number of $\forall$ quantifiers is fixed, then the complexity is $O(|Q||A|^k)$.

Since nonemptiness of NFH is undecidable, so are its universality and containment problems. However, we show that containment is decidable for the fragments that we consider.

Theorem 14. The containment problems of $\text{NFH}_\exists$ and $\text{NFH}_\forall$ in $\text{NFH}_\exists$ and $\text{NFH}_\forall$ and of $\text{NFH}_{3\forall}$ in $\text{NFH}_3$ and $\text{NFH}_{3\forall}$ are PSPACE-complete.

Proof Sketch. The lower bound follows from the PSPACE-hardness of the containment problem for NFH. For the upper bound, for two NFH $A_1$ and $A_2$, we have that $L(A_1) \subseteq L(A_2)$ iff $L(A_1) \cap \overline{L(A_2)} = \emptyset$. We can use the constructions in the proof of Theorem 8 to compute a matching NFH $A = A_1 \cap \overline{A_2}$, and check its nonemptiness. Complementing $A_2$ is exponential in its number of states, and the intersection construction is polynomial.

If $A_1 \in \text{NFH}_3$ and $A_2 \in \text{NFH}_\forall$ or vice versa, then $A$ is an NFH$_3$ or NFH$_\forall$, respectively, whose nonemptiness can be decided in space that is logarithmic in $|A|$.

It follows from the construction in the proof of Theorem 8, that the quantification condition of $A$ may be any interleaving of the quantification conditions of the two intersected NFH. Therefore, for the rest of the fragments, we can construct the intersection such that $A$ is an NFH$_{3\forall}$.

The PSPACE upper bound of Theorem 11 is derived from the number of variables and not from the state-space of the NFH. Therefore, while $|A_2|$ is exponential in the number of states of $A_2$, checking the nonemptiness of $A$ is in PSPACE.

6 Learning NFH

In this section, we introduce $L^*$-based learning algorithms for the fragments $\text{NFH}_\forall$ and $\text{NFH}_3$. We first survey the $L^*$ algorithm [2], and then describe the relevant adjustments for our case.
6.1 Angluin’s L∗ Algorithm

L∗ consists of two entities: a learner, who wishes to learn a DFA A for an unknown (regular) language L, and a teacher, who knows L. During the learning process, the learner asks the teacher two types of queries: membership queries (“is the word w in L?”) and equivalence queries (“is A a DFA for L?”).

The learner maintains A in the form of an observation table T of truth values, whose rows D, D · Σ and columns E are sets of words over Σ, where D is prefix-closed, and E is suffix-closed. Initially, D = E = {e}. For a row d and a column e, the entry for T(d, e) is τ if d · e ∈ L. The entries are filled via membership queries. The vector of truth values for row d is denoted row(d).

Intuitively, the rows in D determine the states of A, and the rows in D · Σ determine the transitions of A: the state row(d · σ) is reached from row(d) upon reading σ.

The learner updates T until it is closed, which, intuitively, ensures a full transition relation and consistent, which, intuitively, ensures a deterministic transition relation. If T is not closed or not consistent then more rows or more columns are added to T, respectively.

When T is closed and consistent, the learner constructs A: The states are the rows of D, the initial state is row(e), the accepting states are those in which T(d, e) = τ, and the transition relation is as described above. The learner then submits an equivalence query. If the teacher confirms, the algorithm terminates. Otherwise, the teacher returns a counterexample w ∈ L(A) but w /∈ L (which we call a positive counterexample), or w /∈ L(A) but w ∈ L (which we call a negative counterexample). The learner then adds w and all its suffixes to E, and proceeds to construct the next candidate DFA A.

It is shown in [2] that as long as A is not a DFA for L, it has less states than a minimal DFA for L. Further, every change in the table adds at least one state to A, and at the end there are at least one state to A. Therefore, the procedure is guaranteed to terminate successfully with a minimal DFA A for L.

The correctness of the L∗ algorithm follows from the fact that regular languages have a canonical form, which guarantees a single minimal DFA for a regular language L. To enable an L∗-based algorithm for NFH, and NFH3, we first define canonical forms for these fragments.

6.2 Canonical Forms for the Alternation-Free Fragments

We begin with the basic terms on which our canonical forms are based.

Definition 15. 1. An NFH, $A_\psi$ is sequence complete if for every word w, it holds that $A_\psi$ accepts w iff it accepts every sequence of w.

2. An NFH, $A_3$ is permutation complete if for every word w, it holds that $A_3$ accepts w iff it accepts every permutation of w.

An NFH, $A_\psi$ accepts a hyperword S iff $A_\psi$ accepts every sequence of size k of S. If some sequence is missing from $L(A)$, then removing the rest of the sequences of S from $L(A_\psi)$ does not affect the non-acceptance of S. Therefore, the underlying automata of sequence-complete NFH, only accept necessary sequences. Similarly, an NFH, $A_3$ accepts a hyperword S iff $A_3$ accepts some permutation p of size k of words in S. Adding the rest of the permutations of p to $L(A_3)$ does not affect the acceptance of S. Therefore, the underlying automata of permutation-complete NFH, only reject the necessary permutations of every hyperword. As a conclusion, we have the following.

Lemma 16. 1. Let $A_\psi$ be an NFH, and let $A'_\psi$ be a sequence-complete NFH, over Σ and X such that for every word w, the underlying NFA $A'_\psi$ accepts w iff $A_\psi$ accepts every sequence of w. Then $\mathcal{L}(A_\psi) = \mathcal{L}(A'_\psi)$.

2. Let $A_3$ be an NFH, and let $A'_3$ be a permutation-complete NFH, over Σ and X such that for every word w, the underlying NFA $A'_3$ accepts w iff $A'_3$ accepts all permutations of w. Then $\mathcal{L}(A_3) = \mathcal{L}(A'_3)$.
Next, we show that we can construct a sequence- or permutation-complete NFH for a given NFH_\text{\#} or NFH_\text{v}, respectively. Intuitively, given \mathcal{A}, for every sequence (permutation) \zeta of \{1, \ldots, k\}, we construct an NFA that runs on \mathbf{w}_\zeta, in the same way that \mathcal{A} runs on \mathbf{w}, for every \mathbf{w}. The underlying NFA we construct for the NFH_\text{\#} and NFH_\text{v} are the intersection and union, respectively, of all these NFA.

\textbf{Lemma 17.} Every NFH_\text{\#} (NFH_\text{v}) \mathcal{A} has an equivalent sequence-complete (permutation-complete) NFH_\text{\#} (NFH_\text{v}) \mathcal{A}' over the same set of variables.

Finally, as the following theorem shows, sequence- and permutation-complete NFH offer a unified model for the alternation-free fragments.

\textbf{Theorem 18.} Let \mathcal{A}_1 and \mathcal{A}_2 be two sequence-complete (permutation-complete) NFH_\text{\#} (NFH_\text{v}) over the same set of variables. Then \Sigma(\mathcal{A}_1) = \Sigma(\mathcal{A}_2) if \& only if \mathcal{L}(\mathcal{A}_1) = \mathcal{L}(\mathcal{A}_2).

Regular languages have a canonical form, which are minimal DFA. We use this property to define canonical forms for NFH_\text{\#} and NFH_\text{v} as sequence-complete (permutation-complete) NFH_\text{\#} with a minimal number of variables and a minimal underlying DFA.

\section{Learning NFH_\text{\#} and NFH_\text{v}}

We now describe our \text{L}^*-based learning algorithms for NFH_\text{\#} and NFH_\text{v}. These algorithms aim to learn an NFH with the canonical form defined in Section 6.2 for a target hyperlanguage \Sigma. Figure 4 presents the overall flow of the learning algorithms for both fragments.

In the case of hyperautomata, the membership queries and the counterexamples provided by the teacher consist of hyperwords. Similarly to [8], we assume a teacher that returns a minimal counterexample in terms of size of the hyperword.

During the procedure, the learner maintains an NFH \mathcal{A} via an observation table for \mathcal{A}, over the alphabet \hat{\Sigma} = (\Sigma \cup \{\#\})^k, where \(k\) is initially set to 0. When the number of variables is increased to \(k' > k\), the alphabet of \mathcal{A} is extended accordingly to \((\Sigma \cup \{\#\})^{k'}\). To this end, we define a function \(\uparrow_k: (\Sigma \cup \{\#\})^k \rightarrow (\Sigma \cup \{\#\})^{k'}\), which replaces every letter \((\sigma_1, \ldots, \sigma_k)\), with \((\sigma_1, \ldots, \sigma_k) + (\sigma_k)^{k' - k}\). That is, the last letter is duplicated to create a \(k'\)-tuple. We extend \(\uparrow_k\) to words: \(\uparrow_k'(w)\) is obtained by replacing every letter \(\sigma\) in \(w\) with \(\uparrow_k(\sigma)\). Notice that, for both fragments, if \(\text{unzip}(d \cdot e) \in \Sigma(\mathcal{A})\), then \(\text{unzip}(\uparrow_k'(d \cdot e)) \in \Sigma(\mathcal{A})\). Accordingly, when the number of variables is increased, every word \(w\) in the rows and columns of \(T\) is replaced with \(\uparrow_k'(w)\), an action which we denote by \(\uparrow_k'(T)\).

\subsection{Learning NFH_\text{\#}}

In the case of NFH_\text{\#}, when the teacher returns a counterexample \(S\), it holds that if \(|S| > k\), then \(S\) must be positive. Indeed, assume by way of contradiction that \(S\) is negative. Then, for every \(k\) words \(w_1, \ldots, w_k\) in \(S\), it holds that \(\text{zip}(w_1, \ldots, w_k) \in \mathcal{L}(\mathcal{A})\), but \(S \notin \Sigma\). Therefore, in an NFH_\text{\#} \mathcal{A}' for \(\Sigma\), there exists some word of the form \(w = \text{zip}(w_1, \ldots, w_k)\) such that \(w_i \in S\) for \(1 \leq i \leq k\), and \(w \notin \mathcal{L}(\mathcal{A}')\). As a result, \{\(w_1, \ldots, w_k\}\} \notin \Sigma. Since \(\text{zip}(w_1, \ldots, w_k)\) and all its sequences are in \(\mathcal{L}(\mathcal{A}')\), then a smaller counterexample is \{\(w_1, \ldots, w_k\}\}, a contradiction to the minimality of \(S\).

In fact, if \(|S| > k\), then it must be that \(|S| = k + 1\). Indeed, since \(S\) is a positive counterexample, and \(\mathcal{A}\) accepts all representations of subsets of size \(k\) of \(S\) (otherwise the teacher would return a counterexample of size \(k\)), then there exists a subset \(S' \subseteq S\) of size \(k + 1\) that should be represented, but is not. Therefore, \(S'\) is a counterexample of size \(k + 1\).

When a counterexample \(S\) of size \(k + 1\) is returned, the learner updates \(k \leftarrow k + 1\), updates \(T\) to \(\uparrow_k^{k+1}(T)\), arbitrarily selects a permutation \(\pi\) of the words in \(S\), and adds \(\text{zip}(\pi)\) and all its suffixes to \(E\). In addition, it updates \(D \cdot \hat{\Sigma}\) in accordance with the new updated \(\hat{\Sigma}\), and fills in the missing entries.
When \(|S| \leq k\), then the counterexample is either positive or negative. If \(S\) is positive, then there exists some permutation \(p\) of the words in \(S\) such that \(A\) does not accept \(\text{zip}(p)\) (a permutation and not a proper sequence, or there would be a smaller counterexample). The learner finds such a permutation \(p\), and adds \(\text{zip}(p)\) and all its suffixes to \(E\). Notice that \(\text{zip}(p)\) does not already appear in \(T\), since a membership query would have returned “yes”, and so \(\hat{A}\) would have accepted \(\text{zip}(p)\).

If \(S\) is negative, then \(A\) accepts all sequences of length \(k\) of words in \(S\), though it should not. Then there exists a permutation \(p\) of the words in \(S\) that does not appear in \(T\), and which \(A\) accepts. The learner then finds such a permutation \(p\) and adds \(\text{zip}(p)\) and all its suffixes to \(E\).

If \(p\) is a permutation of the words in \(S\), and \(S\) is a negative counterexample, then \(\text{zip}(p)\) should not be in \(L(\hat{A})\) due to any other hyperword, and if \(S\) is a positive counterexample, then it should be in \(L(\hat{A})\) for every \(S'\) such that \(S \subseteq S'\). Therefore, the above actions by the learner are valid.

When an equivalence query succeeds, then \(A\) is indeed an NFH\(_r\) for \(\mathcal{L}\). However, \(A\) is not necessarily sequence-complete, as \(\hat{A}\) may accept a word \(w = \text{zip}(w_1, \ldots, w_k)\) but not all of its sequences. This check can be performed by the learner directly on \(\hat{A}\). Notice that \(w\) does not occur in \(T\), since a membership query on \(w\) would return “no”. Once it is verified that \(A\) is not sequence-complete, the counterexample \(w\) (and all its suffixes) are added to \(E\), and the procedure returns to the learning loop.

As we have explained above, variables are added only when necessary, and so the output \(\hat{A}\) is indeed an NFH for \(\mathcal{L}\) with minimally many variables. The correctness of \(L^*\) and the minimality of the counterexamples returned by the teacher guarantee that for each \(k' \leq k\), the run learns a minimal deterministic \(\hat{A}\) for hyperwords in \(\mathcal{L}\) that are represented by \(k'\) variables. Therefore, a smaller \(\hat{A}'\) for \(\mathcal{L}\) does not exist, as restricting \(\hat{A}'\) to the first \(k'\) letters in each \(k\)-tuple would produce a smaller underlying automaton for \(k'\) variables, a contradiction.

Example 19. Figure 3 displays the first two stages of learning \(\mathcal{L}(A_3)\) of Figure 2, \(T_0\) displays the initial table, with \(D = E = \{\epsilon\}\,\text{and}\, \hat{\Sigma} = \{a, b, \#\} \), since \(\{a\}, \{b\}, \text{and} \{\epsilon\}\) are all in \(\mathcal{L}(A_3)\), the initial candidate NFH \(A\) includes a single variable, and, following the answers to the membership queries, a single accepting state.

Since \(\mathcal{L}(A_3)\) includes all hyperwords of size 1, which are now accepted by \(A\), the smallest counterexample the teacher returns is of size 2, which, in the example, is \(\{a, b\}\). Table \(T_1\) is then obtained from \(T_0\) by applying \(\uparrow_1\), updating the alphabet \(\hat{\Sigma}\) to \(\{a, b, \#\}^2\), and updating \(D \cdot \hat{\Sigma}\) accordingly. \(T_1\) is filled by submitting membership queries. For example, for \((b, a) \in D \cdot \hat{\Sigma}\) and \((a, b) \in E\), the learner submits a membership query for \(\{ba, ab\}\), to which the teacher answers “no”.

6.3.2 Learning NFH\(_3\)

The learning process for NFH\(_3\) is similar to the one for NFH\(_r\). We briefly describe the differences.
As in NFH_{∀}, relying on the minimality of the counterexamples returned by the teacher guarantees that when a counterexample \( S \) such that \(|S| > k\) is returned, it is a positive counterexample. Indeed, assume by way of contradiction that \( S \) is a negative counterexample of size \( k' \). Since \( \hat{A} \) accepts \( S \), there exists a word \( \text{zip}(w_1, \ldots, w_k) \) in \( \mathcal{L}(\hat{A}) \) such that \( \{w_1, \ldots, w_k\} \subseteq S \). According to the semantics of \( \exists \), if \( \text{zip}(w_1, w_2, \ldots, w_k) \in \mathcal{L}(\hat{A}) \) then \( S \in \mathcal{L}(A) \). Since \( S \not\in \mathcal{L} \), we have that \( \{w_1, \ldots, w_k\} \) is a smaller counterexample, a contradiction.

Therefore, when the teacher returns a counterexample \( S \) of size \( k' > k \), the alphabet \( \hat{\Sigma} \) is extended to \( (\Sigma \cup \{\#\})^{k'} \), and the table \( T \) is updated by \( \uparrow_k \), as is done for NFH_{∀}.

If \(|S| \leq k\), then \( S \) may be either positive or negative. If \( S \) is negative, then there exists some permutation of \( S \) that is accepted by \( \hat{A} \). However, no such permutation is in \( T \), as a membership query would have returned “no”. Similarly, if \( S \) is positive, then there exists no permutation of \( S \) that \( \hat{A} \) accepts. In both cases, the learner chooses a permutation of \( S \) and adds it, and all its suffixes, to \( E \).

As in the case of NFH_{∀}, the success of an equivalence query does not necessarily imply that \( \hat{A} \) is permutation-complete. If \( \hat{A} \) is not permutation-complete, the learner finds a word \( w \) that is a permutation of \( w' \) such that \( w' \in \mathcal{L}(\hat{A}) \) but \( w \not\in \mathcal{L}(\hat{A}) \), and adds \( w \) as a counterexample to \( E \). The procedure then returns to the learning loop.

## 7 Conclusion and Future Work

We have introduced and studied hyperautomata and hyperlanguages, focusing on the basic model of regular hyperlanguages, in which the underlying automaton is a standard NFA. We have shown that regular hyperlanguages are closed under set operations (complementation, intersection, and union) and are capable of expressing important hyperproperties for information-flow security policies over finite traces. We have also investigated fundamental decision procedures such as checking nonemptiness and membership. We have shown that their regular properties allow the learnability of the alternation-free fragments. Fragments that combine the two types of quantifiers prove to be more challenging, and we leave their learnability to future work.

The notion of hyperlanguages, as well as the model of hyperautomata, can be lifted to handle hyperwords that consist of infinite words: instead of an underlying finite automaton, we can use any model that accepts infinite words. In fact, we believe using an underlying alternating Büchi automaton, such hyperautomata can express the entire logic of HyperLTL [6], using the standard Vardi-Wolper construction for LTL [15] as basis. Our complexity results for the various decision procedures for NFH, combined with the complexity results shown in [9], suggest that using hyperautomata would be optimal, complexity-wise, for handling HyperLTL.

Further future directions include studying non-regular hyperlanguages (e.g., context-free), and object hyperlanguages (e.g., trees). Other open problems include a full investigation of the complexity of decision procedures for alternating fragments of NFH.
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Appendix

A Proofs

Theorem 8

Proof. Complementation. Let $A$ be an NFH. The NFA $\tilde{A}$ can be complemented with respect to its language over $\tilde{\Sigma}$ to an NFA $\tilde{A}$. Then for every assignment $v : X \rightarrow S$, it holds that $\tilde{A}$ accepts $\text{zip}(v)$ iff $\tilde{A}$ does not accept $\text{zip}(v)$. Let $\bar{\alpha}$ be the quantification condition obtained from $\alpha$ by replacing every $\exists$ with $\forall$ and vice versa. We can prove by induction on $\alpha$ that $A$, the NFH whose underlying NFA is $\tilde{A}$, and whose quantification condition is $\bar{\alpha}$, accepts $L(A)$. The size of $A$ is exponential in $|Q|$, due to the complementation construction for $\tilde{A}$.

Now, let $A_1 = \langle \Sigma, X, Q, Q_0, \delta_1, F_1, \alpha_1 \rangle$ and $A_2 = \langle \Sigma, Y, P, P_0, \delta_2, F_2, \alpha_2 \rangle$ be two NFH with $|X| = k$ and $|Y| = k'$ variables, respectively.

Union. We construct an NFH $A_{12} = \langle \Sigma, X \cup Y, Q \cup P \cup \{p_1, p_2\}, Q_0 \cup P_0, \delta, F_1 \cup F_2 \cup \{p_1, p_2\}, \alpha \rangle$, where $\alpha = \alpha_1 \alpha_2$ (that is, we concatenate the two quantification conditions), and where $\delta$ is defined as follows.

- For every $q \in F_1$, we set
  
  \[
  (q \xrightarrow{t+(\sigma_1, \ldots, \sigma_{k'})} p_1) \in \delta
  \]

  and

  \[
  (p_1 \xrightarrow{t+(\sigma_1, \ldots, \sigma_{k'})} p_1) \in \delta
  \]

  for every $t \in (\Sigma \cup \{\#\})^{k'}$.

- For every $q \in F_2$, we set
  
  \[
  (q \xrightarrow{t+(\sigma_1, \ldots, \sigma_{k'})} p_2) \in \delta
  \]

  and

  \[
  (p_2 \xrightarrow{t+(\sigma_1, \ldots, \sigma_{k'})} p_2) \in \delta
  \]

  for every $t \in (\Sigma \cup \{\#\})^{k'}$.
Let $S$ be a hyperword. For every $v : (X \cup Y) \to S$, it holds that if $\text{zip}(v|X) \in \mathcal{L}(\hat{A}_1)$, then $\text{zip}(v) \in \mathcal{L}(\hat{A}_2)$. Indeed, according to our construction, every word assigned to the $Y$ variables is accepted in the $A_1$ component of the construction, and so it satisfies both types of quantifiers. A similar argument holds for $v|_Y$ and $A_2$.

Also, according to our construction, for every $v : (X \cup Y) \to S$, if $\text{zip}(v) \in \mathcal{L}(\hat{A}_2)$, then either $\text{zip}(v|X) \in \mathcal{L}(\hat{A}_1)$, or $\text{zip}(v|Y) \in \mathcal{L}(\hat{A}_2)$. As a conclusion, we have that $\mathcal{L}(A_i) = \mathcal{L}(A_1) \cup \mathcal{L}(A_2)$.

The state space of $A_{ij}$ is linear in the state spaces of $A_1$, $A_2$. However, the size of the alphabet of $A_{ij}$ may be exponentially larger than that of $A_1$ and $A_2$, since we augment each letter with all sequences of size $k'$ (in $A_1$) and $k$ (in $A_2$).

**Intersection.** The proof follows the closure under union and complementation. However, we also offer a direct translation, which avoids the need to complement. We construct an NFH $A_{\gamma} = (\Sigma, X \cup Y, (Q \cup \{q\} \times P \cup \{p\}), (Q_0 \times P_0), \delta, (F_1 \cup \{q\}) \times (F_2 \cup \{p\}), \alpha_1 \alpha_2)$, where $\delta$ is defined as follows.

= For every $(q_1 \xrightarrow{(\sigma_1,\ldots,\sigma_k)} q_2) \in \delta_1$ and every $(p_1 \xrightarrow{(\sigma_1',\ldots,\sigma_{k'})} p_2) \in \delta_2$, we have

$$
\left((q_1, p_1) \xrightarrow{(\sigma_1,\ldots,\sigma_k,\sigma_1',\ldots,\sigma_{k'})} (q_2, p_2)\right) \in \delta
$$

= For every $q_1 \in F_1$, $(p_1 \xrightarrow{(\sigma_1',\ldots,\sigma_{k'})} p_2) \in \delta_2$ we have

$$
\left((q_1, p_1) \xrightarrow{(\#k'+(\sigma_1',\ldots,\sigma_{k'}))} (q, p_2)\right), \left((q, p_1) \xrightarrow{(\#k')+(\sigma_1',\ldots,\sigma_{k'})} (q, p_2)\right) \in \delta
$$

= For every $(q_1 \xrightarrow{(\sigma_1,\ldots,\sigma_k)} q_2) \in \delta_1$ and $p_1 \in F_2$, we have

$$
\left((q_1, p_1) \xrightarrow{(\sigma_1,\ldots,\sigma_k)+(#k')} (q_2, p)\right), \left((q_1, p) \xrightarrow{(\sigma_1',\ldots,\sigma_{k'})+(#k')} (q_2, p)\right) \in \delta
$$

Intuitively, the role of $q, p$ is to keep reading $(\#)^{k'}$ and $(\#)^{k}$ after the word read by $\hat{A}_1$ or $\hat{A}_2$, respectively, has ended.

The NFH $\hat{A}_i$ simultaneously reads two words $\text{zip}(w_1, w_2, \ldots, w_k)$ and $\text{zip}(w'_1, w'_2, \ldots, w'_{k'})$ that are read along $\hat{A}_1$ and $\hat{A}_2$, respectively, and accepts iff both words are accepted. The correctness follows from the fact that for $v : (X \cup Y) \to S$, we have that $\text{zip}(v)$ is accepted by $\hat{A}$ iff $\text{zip}(v|X)$ and $\text{zip}(v|Y)$ are accepted by $\hat{A}_1$ and $\hat{A}_2$, respectively.

This construction is polynomial in the sizes of $A_1$ and $A_2$.

**Theorem 9**

**Proof.** We mimic the proof idea in [9], which uses a reduction from the Post correspondence problem (PCP). A PCP instance is a collection $C$ of dominoes of the form:

$$
\left\{ \begin{array}{c}
\left[ \begin{array}{c}
0_1 \\
1_1
\end{array} \right],
\left[ \begin{array}{c}
0_2 \\
1_2
\end{array} \right],
\ldots,
\left[ \begin{array}{c}
0_k \\
1_k
\end{array} \right]
\end{array} \right\}
$$

where for all $i \in [1, k]$, we have $v_i, u_i \in \{a, b\}^*$. The problem is to decide whether there exists a finite sequence of the dominoes of the form

$$
\left[ \begin{array}{c}
0_{i_1} \\
1_{i_1}
\end{array} \right],
\left[ \begin{array}{c}
0_{i_2} \\
1_{i_2}
\end{array} \right],
\ldots,
\left[ \begin{array}{c}
0_{i_m} \\
1_{i_m}
\end{array} \right]
$$

where each index $i_j \in [1, k]$, such that the upper and lower finite strings of the dominoes are equal, i.e.,

$$
u_{i_1} u_{i_2} \cdots u_{i_m} = v_{i_1} v_{i_2} \cdots v_{i_m}$$
For example, if the set of dominoes is

\[ C_{\text{exmp}} = \left\{ \left[ \begin{array}{c} ab \\ b \end{array} \right], \left[ \begin{array}{c} ba \\ a \end{array} \right], \left[ \begin{array}{c} a \\ aba \end{array} \right] \right\} \]

Then, a possible solution is the following sequence of dominoes from \( C_{\text{exmp}} \):

\[ \text{sol} = \left[ \begin{array}{c} a \\ aba \end{array} \right] \left[ \begin{array}{c} ba \\ a \end{array} \right] \left[ \begin{array}{c} ab \\ b \end{array} \right]. \]

Given an instance \( C \) of PCP, we encode a solution as a word \( w_{\text{sol}} \) over the following alphabet:

\[ \Sigma = \left\{ \sigma \sigma' \mid \sigma,\sigma' \in \{a,b,\hat{a},\hat{b},\$\} \right\}. \]

Intuitively, \( \sigma \) marks the beginning of a new domino, and \( \$ \) marks the end of a sequence of the upper or lower parts of the dominoes sequence.

We note that \( w_{\text{sol}} \) encodes a legal solution iff the following conditions are met:

1. For every \( \frac{\sigma}{\sigma'} \) that occurs in \( w_{\text{sol}} \), it holds that \( \sigma,\sigma' \) represent the same domino letter (both \( a \) or both \( b \), either dotted or undotted).
2. The number of dotted letters in the upper part of \( w_{\text{sol}} \) is equal to the number of dotted letters in the lower part of \( w_{\text{sol}} \).
3. \( w_{\text{sol}} \) starts with two dotted letters, and the word \( u_i \) between the \( i \)th and \( i+1 \)th dotted letters in the upper part of \( w_{\text{sol}} \), and the word \( v_i \) between the corresponding dotted letters in the lower part of \( w_{\text{sol}} \) are such that \( \left\lfloor \frac{u_i}{v_i} \right\rfloor \in C \), for every \( i \).

We call a word that represents the removal of the first \( k \) dominoes from \( w_{sol} \) a partial solution, denoted by \( w_{sol,k} \). Note that the upper and lower parts of \( w_{sol,k} \) are not necessarily of equal lengths (in terms of \( a \) and \( b \) sequences), since the upper and lower parts of a domino may be of different lengths, and so we use letter \( \$ \) to pad the end of the encoding in the shorter of the two parts.

We construct an NFH \( \mathcal{A} \), which, intuitively, expresses the following ideas: (1) There exists an encoding \( w_{sol} \) of a solution to \( C \), and (2) For every \( w_{sol,k} \neq \epsilon \) in a hyperword \( S \) accepted by \( \mathcal{A} \), the word \( w_{sol,k+1} \) is also in \( S \).

\( \mathcal{L}(\mathcal{A}) \) is then the set of all hyperwords that contain an encoded solution \( w_{sol} \), as well as all its suffixes obtained by removing a prefix of dominoes from \( w_{sol} \). This ensures that \( w_{sol} \) indeed encodes a legal solution. For example, a matching hyperword \( S \) (for solution \( sol \) discussed earlier) that is accepted by \( \mathcal{A} \) is:

\[ S = \left\{ w_{sol} = \hat{a} \hat{b} a \hat{a} b, w_{sol,1} = \hat{b} a \hat{b} a \hat{b} b, w_{sol,2} = \hat{a} \hat{b} \hat{b} b \$ \right\}. \]

Thus, the acceptance condition of \( \mathcal{A} \) is \( \alpha = \forall x_1 \exists x_2 \exists x_3 \), where \( x_1 \) is to be assigned a potential partial solution \( w_{sol,k} \), and \( x_2 \) is to be assigned \( w_{sol,k+1} \), and \( x_3 \) is to be assigned \( w_{sol} \).

During a run on a hyperword \( S \) and an assignment \( v : \{x_1, x_2, x_3\} \to S \), the NFH \( \mathcal{A} \) checks that the upper and lower letters of \( w_{sol} \) all match. In addition, \( \mathcal{A} \) checks that the first domino of \( v(x_1) \) is indeed in \( C \), and that \( v(x_2) \) is obtained from \( v(x_1) \) by removing the first tile. \( \mathcal{A} \) performs the latter task by checking that the upper and lower parts of \( v(x_2) \) are the upper and lower parts of \( v(x_1) \) that have been “shifted” back appropriately. That is, if the first tile in \( v(x_2) \) is the encoding of \( \left\lfloor \frac{u_1}{v_1} \right\rfloor \), then \( \mathcal{A} \) uses states to remember, at each point, the last \( |w_i| \) letters of the upper part of \( v(x_2) \) and the last \( |v_i| \) letters of the lower part of \( v(x_2) \), and verifies, at each point, that the next letter in \( v(x_1) \) matches the matching letter remembered by the state.
**Theorem 10**

**Proof.** The lower bound for both fragments follows from the NL-hardness of the nonemptiness problem for NFA.

We turn to the upper bound, and begin with NFH$_3$. Let $A_3$ be an NFH$_3$. We claim that $A_3$ is nonempty iff $\hat{A}_3$ accepts some legal word $w$. The first direction is trivial. For the second direction, let $w \in L(\hat{A}_3)$, and let $S = \text{unzip}(w)$. By assigning $v(x_i) = w[i]$ for every $x_i \in X$, we get $\text{zip}(v) = w$, and according to the semantics of $\exists$, we have that $A_3$ accepts $S$. To check whether $A_3$ accepts a legal word, we can run a reachability check on-the-fly, while advancing from a letter $\sigma$ to the next letter $\sigma'$ only if $\sigma'$ contains $\#$ in all the positions in which $\sigma$ contains $\#$. While each transition $T = q (\sigma_1, \ldots, \sigma_n) \rightarrow p$ in $\hat{A}$ is of size $k$, we can encode $T$ as a set of size $k$ of encodings of transitions of type $q \xrightarrow{\sigma} p$ with a binary encoding of $p, q, \sigma$, as well as $i, t$, where $t$ marks the index of $T$ within the set of transitions of $A$. Therefore, the reachability test can be performed within space that is logarithmic in the size of $A_3$.

Now, let $A_\forall$ be an NFH$_\forall$ over $X$. We claim that $A_\forall$ is nonempty iff $A_\forall$ accepts a hyperword of size 1. For the first direction, let $S \in L(A_\forall)$. Then, by the semantics of $\forall$, we have that for every assignment $\nu : X \rightarrow S$, it holds that $\text{zip}(\nu) \in L(\hat{A}_\forall)$. Let $w \in S$, and let $\nu_u(x_i) = u$ for every $x_i \in X$. Then, in particular, $\text{zip}(\nu_u) \in L(\hat{A}_\forall)$.

To check whether $A_\forall$ accepts a hyperword of size 1, we restrict the reachability test on $\hat{A}_\forall$ to $k$-tuples of the form $(\sigma, \ldots, \sigma)$ for $\sigma \in \Sigma$.

**Theorem 11**

**Proof.** We begin with the upper bound. Let $S \in L(A)$. Then, according to the semantics of the quantifiers, there exist $w_1, \ldots, w_m \in S$, such that for every assignment $v : X \rightarrow S$ in which $v(x_i) = w_i$ for every $1 \leq i \leq m$, it holds that $\hat{A}$ accepts $\text{zip}(v)$. Let $v : X \rightarrow S$ be such an assignment. Then, $\hat{A}$ accepts $\text{zip}(\nu_\zeta)$ for every sequence $\zeta$ of the form $(1, 2, \ldots, m, i_1, i_2, \ldots, i_{k-m})$. In particular, it holds for such sequences in which $1 \leq i_j \leq m$ for every $1 \leq j \leq k - m$, that is, sequences in which the last $k - m$ variables are assigned words that are assigned to the first $m$ variables. Therefore, again by the semantics of the quantifiers, we have that $\{v(x_1), \ldots, v(x_m)\}$ is in $L(A)$. The second direction is trivial.

We call $\text{zip}(\nu_\zeta)$ as described above a witness to the nonemptiness of $A$, i.e., $\text{zip}(\nu_\zeta)$ is an instantiation of the existential quantifiers. We construct an NFA $A$ based on $\hat{A}$ that is nonempty iff $\hat{A}$ accepts a witness to the nonemptiness of $A$. Let $\Gamma$ be the set of all sequences of the above form. For every sequence $\zeta = (i_1, i_2, \ldots, i_k)$ in $\Gamma$, we construct an NFA $A_\zeta = (\hat{\Sigma}, Q, Q_0, \delta_\zeta, F)$, where for every $w \xrightarrow{\sigma_1, \sigma_2, \ldots, \sigma_{k-1}} q'$ in $\delta$, we have $w \xrightarrow{\sigma_1, \sigma_2, \ldots, \sigma_k} q'$ in $\delta_\zeta$. Intuitively, $A_\zeta$ runs on every word $w$ the same way that $\hat{A}$ runs on $w_\zeta$. Therefore, $\hat{A}$ accepts a witness $w$ to the nonemptiness of $A$ iff $w \in L(A_\zeta)$ for every $\zeta \in \Gamma$.

We define $A = \bigcap_{\zeta \in \Gamma} A_\zeta$. Then $\hat{A}$ accepts a witness to the nonemptiness of $A$ iff $A$ is nonempty. Since $|\Gamma| = m^{k-m}$, the state space of $A$ is of size $O(n^{m^{k-m}})$, where $n = |Q|$, and its alphabet is of size $|\hat{\Sigma}|$. Notice that for $A$ to be nonempty, $\delta$ must be of size at least $|\hat{\Sigma}|^{(k-m)}$, to account for all the permutations of letters in the words assigned to the variables under $\forall$ quantifiers (otherwise, we can immediately return “empty”). Therefore, $|A|$ is $O(n \cdot |\hat{\Sigma}|^k)$. We then have that the size of $A$ is $O(|\hat{A}|^k)$. If the number $k - m$ of $\forall$ quantifiers is fixed, then $m^{k-m}$ is polynomial in $k$. However, now $|A|$ may be polynomial in $n, k$, and $|\hat{\Sigma}|$, and so in this case as well, the size of $A$ is $O(|\hat{A}|^k)$.

Since the nonemptiness problem for NFA is NL-complete, the problem for NFH$_{2^k}$ can be decided.
in space of size that is polynomial in \(|\hat{A}|\).

**PSPACE hardness** For the lower bound, we show a reduction from a polynomial version of the **corridor tiling problem**, defined as follows. We are given a finite set \(T\) of tiles, two relations \(V \subseteq T \times T\) and \(H \subseteq T \times T\), an initial tile \(t_0\), a final tile \(t_f\), and a bound \(n > 0\). We have to decide whether there is some \(m > 0\) and a tiling of an \(n \times m\)-grid such that (1) The tile \(t_0\) is in the bottom left corner and the tile \(t_f\) is in the top right corner, (2) A horizontal condition: every pair of horizontal neighbors is in \(H\), and (3) A vertical condition: every pair of vertical neighbors is in \(V\). When \(n\) is given in unary notation, the problem is known to be PSPACE-complete.

Given an instance \(C\) of the tiling problem, we construct an NFH \(A\) that is nonempty iff \(C\) has a solution. We encode a solution to \(C\) as a word \(w_{sol} = w_1 \cdot w_2 \cdot w_m \$\) over \(\Sigma = T \cup \{1, 2, \ldots, n, \$\}\), where the word \(w_i\), of the form \(1 \cdot t_{1,i} \cdot 2 \cdot t_{2,i} \cdot \ldots \cdot n \cdot t_{n,i}\), describes the contents of row \(i\).

To check that \(w_{sol}\) indeed encodes a solution, we need to make sure that:

1. \(w_1\) begins with \(t_0\) and \(w_m\) ends with \(t_f\$\).
2. \(w_i\) is of the correct form.
3. Within every \(w_i\), it holds that \((t_{j,i}, t_{j+1,i}) \in H\).
4. For \(w_1, w_{i+1}\), it holds that \((t_{j,i}, t_{j,i+1}) \in V\) for every \(1 \leq j \leq n\).

Verifying items 1 – 3 is easy via an NFA of size \(O(n|H|)\). The main obstacle is item 4.

We describe an NFH \(A = \langle T \cup \{0, 1, 2, \ldots, n, \$\}, \{y_1, y_2, y_3, x_1, \ldots, x_{\log(n)}\}, Q, \{q_0\}, \delta, F, \alpha\rangle\) that is nonempty iff there exists a word that satisfies items 1 – 4. The quantification condition \(\alpha\) is \(\exists y_1 \exists y_2 \exists y_3 \forall x_1 \ldots \forall x_{\log(n)}\). The NFH \(A\) only proceeds on letters whose first three positions are of the type \((r, 0, 1)\), where \(r \in T \cup \{1, 2, \ldots, n, \$\}\). Notice that this means that \(A\) requires the existence of the words \(0||w_{sol}|\) and \(1||w_{sol}|\) (the 0 word and 1 word, henceforth). \(A\) makes sure that the word assigned to \(y_1\) matches a correct solution w.r.t. items 1 – 3 described above. We proceed to describe how to handle the requirement for \(V\). We need to make sure that for every position \(j\) in a row, the tile in position \(j\) in the next row matches the current one w.r.t. \(V\). We can use a state \(q_j\) to remember the tile in position \(j\), and compare it to the tile in the next occurrence of \(j\). The problem is avoiding having to check all positions simultaneously, which would require exponentially many states. To this end, we use \(\log(n)\) copies of the 0 and 1 words to form a binary encoding of the position \(j\) that is to be remembered. The \(\log(n)\) \(\forall\) conditions make sure that every position within \(1 – n\) is checked.

We limit the checks to words in which \(x_1, \ldots, x_{\log(n)}\) are the 0 or 1 words, by having \(A\) accept every word in which there is a letter that is not over 0, 1 in positions 4, \ldots, \(\log(n)\) + 3. This takes care of accepting all cases in which the word assigned to \(y_3\) is also assigned to one of the \(x\) variables.

To check that \(x_1, \ldots, x_{\log(n)}\) are the 0 or 1 words, \(A\) checks that the values in positions 4 to \(\log(n)\) + 3 remain constant throughout the run. In these cases, upon reading the first letter, \(A\) remembers the value \(j\) that is encoded by the constant assignments to \(x_1, \ldots, x_{\log(n)}\) in a state, and makes sure that throughout the run, the tile that occurs in the assignment \(y_1\) in position \(j\) in the current row matches the tile in position \(j\) in the next row.

We construct a similar reduction for the case that the number of \(\forall\) quantifiers is fixed: instead of encoding the position by \(\log(n)\) bits, we can directly specify the position by a word of the form \(j^*\), for every \(1 \leq j \leq n\). Accordingly, we construct an NFH \(A_{xy}\) over \(\{x, y_1, \ldots, y_n, z\}\), with a quantification condition \(\alpha = \exists x \exists y_1 \ldots \exists y_n \forall z\). The NFA \(A\) advances only on letters whose assignments to \(y_1, \ldots, y_n\) are always 1, 2, \ldots, \(n\), respectively, and checks only words assigned to \(z\) that are some constant \(1 \leq j \leq n\). Notice that the fixed assignments to the \(y\) variables leads to \(\delta\) of polynomial size. In a hyperword accepted by \(A\), the word assigned to \(x\) is \(w_{sol}\), and the word assigned to \(z\) specifies which index should be checked for conforming to \(V\).
Theorem 12

Proof. We can decide the membership of \( S \in \mathcal{L}(A) \) by iterating over all relevant assignments from \( X \) to \( S \), and for every such assignment \( v \), checking on-the-fly whether \( \text{zip}(v) \) is accepted by \( \tilde{A} \). This algorithm uses space of size that is polynomial in \( k \) and logarithmic in \( |A| \) and in \( |S| \).

In the case that \( k' = O(\log k) \), an \( \mathsf{NP} \) upper bound is met by iterating over all assignments to the variables under \( \forall \), while guessing assignments to the variables under \( \exists \). For each such assignment \( v \), checking whether \( \text{zip}(v) \in \mathcal{L}(\tilde{A}) \) can be done on-the-fly.

We show \( \mathsf{NP} \)-hardness for this case by a reduction from the Hamiltonian cycle problem. Given a graph \( G = (V, E) \) where \( V = \{v_1, v_2, \ldots, v_n\} \) and \( |E| = m \), we construct an NFH \( \tilde{A} \) over \( \{0, 1\} \) with \( n \) states, \( n \) variables, \( \delta \) of size \( m \), and a hyperword \( S \) of size \( n \), as follows. \( S = \{w_1, \ldots, w_n\} \), where \( w_i \) is the word over \( \{0, 1\} \) in which all letters are 0 except for the \( i \)’th. The structure of \( \tilde{A} \) is identical to that of \( G \), and we set \( Q_0 = F = \{v_1\} \). For the transition relation, for every \( (v_i, v_j) \in E \), we have \( (v_i, \sigma_i, v_j) \in \delta \), where \( \sigma_i \) is the letter over \( \{0, 1\}^n \) in which all positions are 0 except for position \( i \). Intuitively, the \( i \)’th letter in an accepting run of \( \tilde{A} \) marks traversing \( v_i \). Assigning \( w_j \) to \( x_i \) means that the \( j \)’th step of the run traverses \( v_i \). Since the words in \( \mu \) make sure that every \( v \in V \) is traversed exactly once, and that the run on them is of length \( n \), we have that \( \tilde{A} \) accepts \( S \) iff there exists some permutation \( \rho \) of the words in \( S \) such that \( \rho \) matches a Hamiltonian cycle in \( G \).

Remark. To account for all the assignments to the \( \forall \) variables, \( \delta \) – and therefore, \( \tilde{A} \) – must be of size at least \( 2^k \) (otherwise, we can return “no”). We then have that if \( k = O(k') \), then space of size \( k \) is logarithmic in \( |\tilde{A}| \), and so the problem in this case can be solved within logarithmic space. A matching NL lower bound follows from the membership problem for NFAs.

Theorem 13

Proof. Let \( A = (\Sigma, P, P_0, \rho, F) \) be an NFA, and let \( A = (\Sigma, \{x_1, \ldots, x_k\}, Q, Q_0, \delta, F, \alpha) \) be an NFH.

First, we construct an NFH \( A' = (\Sigma \cup \{\#\}, P', P_0', \rho', F') \) by extending the alphabet of \( A \) to \( \Sigma \cup \{\#\} \), adding a new and accepting state \( p_f \) to \( P \) with a self-loop labeled by \( \# \), and transitions labeled by \( \# \) from every \( q \in F \) to \( p_f \). The language of \( A' \) is then \( \mathcal{L}(A) \cup \{\#\}^* \). We describe a recursive procedure (iterating over \( \alpha \)) for deciding whether \( \mathcal{L}(A) \in \mathcal{L}(\tilde{A}) \).

For the case that \( k = 1 \), it is easy to see that if \( \alpha = \exists x_1 \), then \( \mathcal{L}(A) \in \mathcal{L}(\tilde{A}) \) iff \( \mathcal{L}(A) \cap \mathcal{L}(\tilde{A}) \neq \emptyset \). Otherwise, if \( \alpha = \forall x_1 \), then \( \mathcal{L}(A) \in \mathcal{L}(\tilde{A}) \) iff \( \mathcal{L}(A) \notin \mathcal{L}(\tilde{A}) \), where \( \tilde{A} \) is the NFH for \( \mathcal{L}(A) \) described in Theorem 8. Notice that the quantification condition for \( \tilde{A} \) is \( \exists x_1 \), and so this conforms to the base case.

For \( k > 1 \), we construct a sequence of NFHs \( A_1, A_2, \ldots, A_k \). If \( Q_1 = \exists \) then we set \( A_1 = A \), and otherwise we set \( A_1 = \tilde{A} \). Let \( A_i = (\Sigma, \{x_1, \ldots, x_k\}, Q_i, Q_0, \delta_i, F_i, \alpha_i) \). If \( \alpha_i \) starts with \( \exists \), then we construct \( A_{i+1} \) as follows.

The set of variables of \( A_{i+1} \) is \( \{x_{i+1}, \ldots, x_k\} \), and the quantification condition \( \alpha_{i+1} \) is \( Q_{i+1} x_{i+1} \cdots Q_k x_k \), for \( \alpha_i = Q_i x_i Q_{i+1} \cdots Q_k x_k \). The set of states of \( A_{i+1} \) is \( Q_{i} \times P' \), and the set of initial states is \( Q_0' \times P_0 \). The set of accepting states is \( F_i \times F' \). For every \( (q, (\sigma_{i+1} \cdots \sigma_k)) \) \( \in \delta_i \) and every \( (p, (q', p')) \in \rho \), we have \( (q, p) \mapsto (q', p') \in \delta_{i+1} \). Then, \( \tilde{A}_{i+1} \) accepts a word \( \text{zip}(u_1, u_2, \ldots, u_{k-1}) \) iff there exists a word \( w \in \mathcal{L}(A) \), such that \( \tilde{A}_i \) accepts \( \text{zip}(u_1, u_2, \ldots, u_{k-1}) \).

Let \( v : \{x_1, \ldots, x_k\} \rightarrow A \). Then \( \mathcal{L}(A) \models v \) \((\alpha_i, A_i) \) iff there exists \( w \in \mathcal{L}(A) \) such that \( \mathcal{L}(A) \models v[x \rightarrow w] \) \((\alpha_{i+1}, A_{i+1}) \). For an assignment \( v' : \{x_{i+1}, \ldots, x_k\} \rightarrow \mathcal{L}(A) \), it holds that \( \text{zip}(v') \) is accepted by \( \tilde{A}_{i+1} \) if and only if there exists a word \( w \in \mathcal{L}(A) \) such that \( \text{zip}(v) \in \mathcal{L}(A) \), where \( v \) is obtained from \( v' \) by setting \( v(x_{i+1}) = w \). Therefore, we have that \( \mathcal{L}(A) \models v[x \rightarrow w] \) \((\alpha_i, A_i) \) iff \( \mathcal{L}(A) \models v' \) \((\alpha_{i+1}, A_{i+1}) \), that is, \( \mathcal{L}(A) \in \mathcal{L}(A_i) \) iff \( \mathcal{L}(A) \in \mathcal{L}(A_{i+1}) \).
Then we begin with NFH. 

Proof. For the lower bound, we show a reduction from the containment problem for NFA, which is known to be PSPACE-hard. Let \( A_1, A_2 \) be NFA. We “convert” them to NFH \( A_1, A_2 \) by adding to both a single variable \( x \), and a quantification condition \( \forall x \). By the semantics of the \( \forall \) quantifier, we have that \( \mathcal{L}(A_1) = \{ S | S \subseteq \mathcal{L}(A_1) \} \), and similarly for \( A_2 \). Therefore, we have that \( \mathcal{L}(A_1) \subseteq \mathcal{L}(A_2) \) iff \( \mathcal{L}(A_1) \subseteq \mathcal{L}(A_2) \).

For the upper bound, first notice that complementing an NFH yields an NFH, and vice versa. Consider two NFH \( A_1 \) and \( A_2 \). Then \( \mathcal{L}(A_1) \subseteq \mathcal{L}(A_2) \) iff \( \mathcal{L}(A_1) \cap \overline{\mathcal{L}(A_2)} = \emptyset \). We can use the constructions in the proof of Theorem 8 to compute a matching NFH \( A = A_1 \cap \overline{A_2} \), and check its nonemptiness. The complementation construction is exponential in \( n \), the number of states of \( A_2 \), and the intersection construction is polynomial in \( |A_1|, |A_2| \).

If \( A_1 \in \text{NFH}_3 \) and \( A_2 \in \text{NFH}_3 \) or vice versa, then \( A \) is an NFH or NFHY, respectively, whose nonemptiness can be decided in space that is logarithmic in \( |A| \).

Now, consider the case where \( A_1 \) and \( A_2 \) are both \( \text{NFH}_3 \) or both \( \text{NFHY} \). It follows from the proof of Theorem 8, that for two NFH \( A, A' \), the quantification condition of \( A \cap A' \) may be any interleaving of the quantification conditions of \( A \) and \( A' \). Therefore, if \( A_1, A_2 \in \text{NFH}_3 \) or \( A_1, A_2 \in \text{NFHY} \), we can construct \( A \) to be an \( \text{NFH}_{3V} \). This is also the case when \( A_1 \in \text{NFH}_{3V} \) and \( A_2 \in \text{NFH}_3 \) or \( A_2 \in \text{NFHY} \).

Either \( A_2 \) or \( \overline{A_2} \) is an NFHY, whose underlying NFA has a transition relation of size that is exponential in \( k \) (otherwise the NFHY is empty). The same holds for \( A_1 \in \text{NFH}_{3V} \). The PSPACE upper bound of Theorem 11 is derived from the number of variables and not from the state-space of the NFH. Therefore, while \( |A_2| \) is exponential in the number of states of \( A_2 \), checking the nonemptiness of \( A \) is in PSPACE.

Lemma 16

Proof. We begin with NFHY. For the first direction, since \( \mathcal{L}(A_\psi) \subseteq \mathcal{L}(A_\psi') \), we have \( \mathcal{L}(A_\psi') \subseteq \mathcal{L}(A_\psi) \). For the second direction, let \( S \in \mathcal{L}(A_\psi) \). Then for every \( v : S \to X \), it holds that \( \text{zip}(v) \in \mathcal{L}(A_\psi) \). Also, \( \text{zip}(v') \in \mathcal{L}(A_\psi) \) for every sequence \( v' \) of \( v \). Then \( \text{zip}(v) \) and all its sequences are in \( \mathcal{L}(A_\psi) \). Since this holds for every \( v : X \to S \), we have that \( S \in \mathcal{L}(A_\psi) \).

We proceed to NFH3. For the first direction, since \( \mathcal{L}(A_3) \subseteq \mathcal{L}(A_3') \), we have \( \mathcal{L}(A) \subseteq \mathcal{L}(A') \). For the second direction, let \( S \in \mathcal{L}(A_3') \). Then there exists \( v : S \to X \) such that \( \text{zip}(v) \in \mathcal{L}(A_3) \). Then \( \text{zip}(v) \) is a permutation of some word \( \text{zip}(v') \in \mathcal{L}(A_3) \). According to the semantics of the \( \exists \) quantifier, we have that \( S \in \mathcal{L}(A_3) \).

Lemma 17

Proof. We begin with NFHY. To construct \( A_\psi' \) given \( A_\psi \), we use a similar construction to the one presented in the proof of Theorem 11. Essentially, for every sequence \( \zeta \) of \( (1, 2, \ldots, k) \), we construct an NFA \( A_\zeta \), in which every run on a word \( w \) matches a run of \( A_\psi \) on \( w_\zeta \). The NFHY \( A' \) is then
obtained from $A_\forall$ by replacing the underlying NFA with $\bigcap_{\zeta \in \Gamma} A_\zeta$, where $\Gamma$ is the set of sequences of $(1, 2, \ldots, k)$.

For NFH$_2$, similarly to the case of NFH$_\forall$, we construct $A'_2$ given $A_3$ by constructing $A_\zeta$ for every permutation $\zeta$ of $(1, 2, \ldots, k)$. In this case, the NFH$_2 A'_2$ is obtained from $A_3$ by replacing the underlying NFA with $\bigcup_{\zeta \in \Gamma} A_\zeta$, where $\Gamma$ is the set of permutations of $(1, 2, \ldots, k)$.

**Theorem 18**

**Proof.** We begin with NFH$_\forall$. For the first direction, let $w \in L(\hat{A}_\forall)$. Since $A_1$ is sequence-complete, then $w' \in L(\hat{A}_1)$ for every sequence $w'$ of $w$. Then, by the semantics of the $\forall$ quantifier, we have that unzip$(w) \in L(A_1)$. Therefore, unzip$(w) \in L(A_2)$, and so $w$ (and all its sequences) are in $L(A_2)$. A similar argument can be made to show that for every $w \in L(A_1)$, it holds that $w \in L(A_1)$. Therefore, $L(A_1) = L(A_2)$. The second direction is trivial.

We continue to NFH$_3$. For the first direction, let $w \in L(\hat{A}_3)$. Then unzip$(w) \in L(A_4)$. Then, by the semantics of the $\exists$ quantifier, there exists some permutation $w'$ of $w$ such that $w' \in L(A_2)$. Since $A_2$ is permutation-complete, we have that $w \in L(A_2)$. A similar argument can be made to show that for every $w \in L(A_2)$, it holds that $w \in L(A_1)$. Therefore, $L(A_1) = L(A_2)$. The second direction is trivial.