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# Schema-Based Automata Determinization

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**Abstract.** We propose an algorithm for schema-based determinization of finite automata on words and of stepwise hedge automata on nested words. The idea is to integrate schema-based cleaning directly into automata determinization. We prove the correctness of our new algorithm and show that it is always more efficient than standard determinization followed by schema-based cleaning. Our implementation permits to obtain a small deterministic automaton for an example of an XPath query, where standard determinization yields a huge stepwise hedge automaton for which schema-based cleaning runs out of memory.

**Keywords:** Automata, trees, nested words, path queries, XPATH.

## 1 Introduction

Schemas and queries for nested words are definitions of languages of words, trees, unranked trees, and hedges. They can model and query structured text documents such as XML and JSON documents.

Regular queries and schemas can be defined by deterministic nested word automaton (*NWA*) [24,8,2,28]. An example for a regular schema is the XML data model and examples for regular queries are the forward navigational XPath queries on *XML* documents. Path queries can be seen as logical queries with a single free variable  $x$ . Such queries define languages of nested words containing exactly one occurrence of  $x$ . This property in turn, can be expressed by a schema  $one^x$  over the alphabet extended by the query's variable  $x$ .

Stepwise hedge automata (*SHAs*) provide alternative definitions for regular schemas and queries on nested words [26]. *SHAs* naturally subsume finite automata on words (*NFAs*) as well as stepwise tree automata for unranked trees [10]. *SHAs* have the same expressive power as *NWAs* modulo P-time transformations. Furthermore, *SHAs* come with a notion of determinism that generalizes on the left-to-right determinism of *NFAs* and on the bottom-up determinism of tree automata. An algorithm for determinizing *SHAs* can be based on the usual subset construction in contrast to *NWAs*. This becomes possible since *SHAs* do not support any form of top-down determinism, which for *NWAs* can be ruled out by imposing the weak single-entry property.

There exist compilers from forward navigational XPath queries to *NWAs* [4,25,12] and to *SHAs* [26]. The resulting automata can be determinized in, at most, exponential time. Deterministic automata are crucial for algorithmic tasks such as universality or inclusion checking. Both problems can be decided in P-time for the classes of deterministic *SHAs* or *NWAs*, but is DEXPTIME

complete in the nondeterministic cases. For instance, universality checking is relevant for the earliest query answering of XPath queries on XML streams [17]. It is also relevant for the efficient enumeration of the answer sets of regular queries [29]. The need for deterministic automata in these applications motivates the question of how to determinize automata for nested words in practice.

Debarbieux et al. [12] noticed that the usual determinization algorithm for *NWAs* often behaves badly when applied to *NWAs* obtained from XPath queries as simple as  $//a/b$ . As recalled in the survey of Okhotin and Salomaa [28], this determinization algorithm was first invented by von Braunmühl and Verbeek in the eighties in the journal version of [8] and then rediscovered various times later on, for instance in [3]. Niehren and Sakho [26,7] observed only recently that the situation is different for the determinization of *SHAs*: It works out nicely for the *SHA* of  $//a/b$  and also for all other *SHAs* obtained by compilation from forward navigational XPath queries in the XPathMark benchmark [16]. Even more surprisingly, the same good behaviour was observed for the determinization algorithm for *NWA* when restricted to *NWAs* with the weak-single entry property. This property failed for the *NWAs* considered by Debarbieux, but could have been established in quadratic time by compiling *NWAs* to *SHAs* forth and back.

We then observed, unfortunately, that the determinization algorithm for *SHAs* may still behave badly when applied to some forward navigational XPath queries, which arise in practice but not in the XPathMark benchmark [16]. A typical killer example is the following XPath query:

(QN7)      `/a/b/( * | @* | comment() | text() )`

It selects all nodes of an XML document that are descendants of a  $b$ -element below an  $a$ -element at the root. The nodes may have any XML type: element, attribute, comment, or text. The nondeterministic *SHA* has 132 states and an overall size of 322. Its determinization however leads to an automaton with 10.003 states and an overall size of 1.633.790.

This size is way too big for many post-processing methods such as schema-based cleaning or *SHA* minimization [26]. The idea of schema-based cleaning [27] is to keep only those rules and states of the automaton for the query, that are used to recognize some nested word that satisfies the schema. So one could not even see, that after cleaning with the schema  $one^x$  and the XML data model, the resulting deterministic *SHA* for QN7 had only 74 states. After minimization, the automaton goes down to 22 states and an overall size of 144.

We therefore propose to integrate schema-based cleaning directly into the determinization algorithm. The idea is to keep only those subsets of states of the query automaton during the determinization, that can be aligned to some state of the schema automaton. As our main theorem, we prove that schema-based determinization always produces the same deterministic automaton than schema-free determinization followed by schema-based cleaning. Its worst case complexity, however, is smaller than that of the determinization followed by schema-based cleaning. In the case of the *SHA* for QN7, the schema-based determinization succeeds in less than a second, while schema-based cleaning is not possible even after a few hours following standard determinization.

**Outline.** In Section 2, we recall for NFAs and discuss how to use them as schemas and queries on words. In Section 3, we recall schema-based cleaning for NFAs.

$$\begin{array}{c}
 \frac{I^A \neq \emptyset}{I^A \in I^{\mathcal{Q}^{\det(A)}} \quad I^A \in \mathcal{Q}^{\det(A)}} \quad \frac{Q \in \mathcal{Q}^{\det(A)} \quad Q \cap F^A \neq \emptyset}{Q \in F^{\det(A)}} \\
 \frac{Q \in \mathcal{Q}^{\det(A)} \quad Q' = \{q' \in \mathcal{Q}^A \mid q \xrightarrow{a} q' \in \Delta^A, q \in Q\} \neq \emptyset}{Q \xrightarrow{a} Q' \in \Delta^{\det(A)} \quad Q' \in \mathcal{Q}^{\det(A)}} \\
 \det(A) = (\Sigma, \mathcal{Q}^{\det(A)}, \Delta^{\det(A)}, I^{\det(A)}, F^{\det(A)})
 \end{array}$$

 Fig. 1: Accessible determinization  $\det(A)$ .

In Section 4, we contribute our schema-based determinization algorithm in the case of NFAs and show its correctness. In Section 5, we recall the notion of *SHAs* for defining languages of nested words. In Section 6, we lift schema-based determinization to *SHAs*. Full proofs are given in the Appendix. It also contains a section on further related work.

## 2 Finite Automata on Words, Schemas, and Queries

In this section, we recall the definition of NFAs and discuss how to use them as schemas and queries on words.

Let  $\mathbb{N}$  be the set of natural numbers including 0. The set of words over a finite alphabet  $\Sigma$  is  $\Sigma^* = \bigcup_{n \in \mathbb{N}} \Sigma^n$ . A word  $(a_1, \dots, a_n) \in \Sigma^n$  is written as  $a_1 \dots a_n$ . We denote by  $\varepsilon$  the empty word, i.e., the unique element of  $\Sigma^0$  and by  $w_1 \cdot w_2 \in \Sigma^*$  the concatenation of two words  $w_1, w_2 \in \Sigma^*$ . For example, if  $\Sigma = \{a, b\}$  then  $aa \cdot bb = aabb = a \cdot a \cdot b \cdot b$ .

**Definition 1.** A NFA is a tuple  $A = (\Sigma, \mathcal{Q}, \Delta, I, F)$  such that  $\mathcal{Q}$  is a finite set of states, the alphabet  $\Sigma$  is a finite set,  $I, F \subseteq \mathcal{Q}$  are subsets of initial and final states, and  $\Delta \subseteq \mathcal{Q} \times \Sigma \times \mathcal{Q}$  is the set of transition rules.

The size of a NFA is  $|A| = |\mathcal{Q}| + |\Delta|$ . A transition rule  $(q, a, q') \in \Delta$  is denoted by  $q \xrightarrow{a} q' \in \Delta$ . We define transitions  $q \xrightarrow{w} q'$  wrt  $\Delta$  for arbitrary words  $w \in \Sigma^*$  between states  $q, q' \in \mathcal{Q}$  by the following inference rules:

$$\frac{q \in \mathcal{Q}}{q \xrightarrow{\varepsilon} q \text{ wrt } \Delta} \quad \frac{q \xrightarrow{a} q' \in \Delta}{q \xrightarrow{a} q' \text{ wrt } \Delta} \quad \frac{q_0 \xrightarrow{w_1} q_1 \text{ wrt } \Delta \quad q_1 \xrightarrow{w_2} q_2 \text{ wrt } \Delta}{q_0 \xrightarrow{w_1 \cdot w_2} q_2 \text{ wrt } \Delta}$$

The language of words recognized by a NFA then is  $\mathcal{L}(A) = \{w \in \Sigma^* \mid q \xrightarrow{w} q' \text{ wrt } \Delta, q \in I, q' \in F\}$ . A NFA  $A$  is called *deterministic* or equivalently a DFA, if it has at most one initial state, and for every pair  $(q, a) \in \mathcal{Q} \times \Sigma$  there is at most one state  $q' \in \mathcal{Q}^A$  such that  $q \xrightarrow{a} q' \in \Delta^A$ .

Any NFA  $A$  can be converted into a DFA that recognizes the same language by the usual subset construction. The accessible determinization  $\det(A)$  of  $A = (\Sigma, \mathcal{Q}^A, \Delta^A, I^A, F^A)$  is defined by the inference rules in Fig. 1. It works like the usual subset construction, except that only accessible subsets are created. It is well known that  $\mathcal{L}(A) = \mathcal{L}(\det(A))$ . Since only accessible subsets of states are

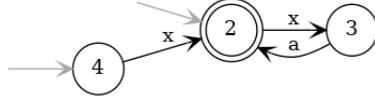


Fig. 2: The NFA  $A_0$  for the regular expression  $(x + \varepsilon).(x.a)^*$

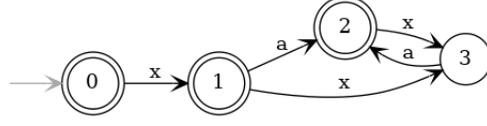


Fig. 3: The accessible determinization  $\det(A_0)$  up to the renaming of states  $[\{2, 4\}/0, \{2, 3\}/1, \{2\}/2, \{3\}/3]$ .

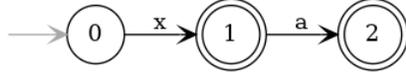


Fig. 4: The schema-based cleaning of  $\det(A_0)$  with schema  $words-one_x^{\Sigma}$ .

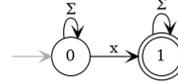


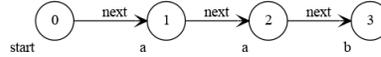
Fig. 5: Schema  $words-one_x^{\Sigma}$  with alphabet  $\Sigma \uplus \{x\}$ .

added, we have  $\mathcal{Q}^{\det(A)} \subseteq 2^{\mathcal{Q}^A}$ . Therefore, the accessible determinization may even reduce the size of the automaton and often avoid the exponential worst case where  $\mathcal{Q}^{\det(A)} = 2^{\mathcal{Q}^A}$ .

**Proposition 2.** *The accessible determinization  $\det(A)$  of a NFA  $A$  can be computed in expected amortized time  $O(|\mathcal{Q}^{\det(A)}| |\Delta^A| + |A|)$ .*

As a running example, we consider the NFA  $A_0$  for the regular expression  $(x + \varepsilon).(x.a)^*$  that is drawn as a labeled digraph in Fig. 2: the nodes of the graph are the states and the labeled edges represent the transitions rules. The initial states are indicated by an ingoing arrow and the final state are doubly circled. The graph of the DFA  $\det(A_0)$  obtained by accessible determinization is shown in Fig. 3. It is given up to a renaming of the states that is given in the caption. Note that only 4 out of the  $2^3 = 8$  subsets are accessible, so the size increases only by a single state and two transitions rules in this example.

A *regular schema* over  $\Sigma$  is a DFA with the alphabet  $\Sigma$ . We next show how to use automata to define regular queries on words. For this, any word is seen as a labeled digraph. The labeled digraph of the word  $aab$ , for instance, is drawn to the right. The set of nodes of



the graph is the set of positions of the word  $pos(w) = \{0, \dots, n\}$  where  $n$  is the length of  $w$ . Position 0 is labeled by *start*, while all other positions are labeled by a single letter in  $\Sigma$ . A monadic query function on words with alphabet  $\Sigma$  is a total function  $\mathbf{Q}$  that maps some words  $w \in \Sigma^*$  to a subset of position  $\mathbf{Q}(w) \subseteq pos(w)$ . We say that a position  $\pi \in pos(w)$  is selected by  $\mathbf{Q}$  if  $w \in dom(\mathbf{Q})$  and  $\pi \in \mathbf{Q}(w)$ .

Let us fix a single variable  $x$ . Given a position  $\pi$  of a word  $w \in \Sigma^*$  let  $w * [\pi/x]$  be the word obtained from  $w$  by inserting  $x$  after position  $\pi$ . We note that all words of the form  $w * [\pi/x]$  contain a single occurrence of  $x$ . Such words are also called  $V$ -structures where  $V = \{x\}$  (see e.g [30]).

The set of all  $V$ -structures can be defined by the schema  $words-one_x^{\Sigma}$  over  $\Sigma \uplus \{x\}$  in Fig. 5. It is natural to identify any total monadic query function

$\mathbf{Q}$  with the language of  $V$ -structures  $L_{\mathbf{Q}} = \{w * [\pi/x] \mid w \in \Sigma^*, \pi \in \mathbf{Q}(w)\}$ . This view permits us to define a subclass of total monadic query functions by automata.

A (*monadic*) *query automaton* over  $\Sigma$  is a NFA  $A$  with alphabet  $\Sigma \uplus \{x\}$ . It defines the unique total monadic query function  $\mathbf{Q}$  such that  $L_{\mathbf{Q}} = \mathcal{L}(A) \cap \mathcal{L}(\text{words-one}_{\Sigma}^x)$ . A position  $\pi$  of a word  $w \in \Sigma^*$  is thus selected by the query  $\mathbf{Q}$  on  $w$  if and only if the  $V$ -structure  $w * [\pi/x]$  is recognized by  $A$ , i.e.:

$$\pi \in \mathbf{Q}(w) \Leftrightarrow w * [\pi/x] \in \mathcal{L}(A)$$

A query function is called regular if it can be defined by some NFA. It is well-known from the work of Büchi in the sixties [9] that the same class of regular query functions can be defined equivalently by monadic second-order logic.

We note that only the words satisfying the schema  $\text{words-one}_{\Sigma}^x$  (the  $V$ -structures) are relevant for the query function  $\mathbf{Q}$  of a query automaton  $A$ . The query automaton  $A_0$  in Fig. 2 for instance, defines the query function that selects the start position of the words  $\varepsilon$  and  $a$  and no other positions elsewhere. This is since the subset of  $V$ -structures recognized by  $A_0$  is  $x + x.a$ . Note that the words  $\varepsilon$  and  $xxa$  do also belong to  $\mathcal{L}(A_0)$ , but are not  $V$ -structures, and thus are irrelevant for the query function  $\mathbf{Q}$ .

### 3 Schema-Based Cleaning

Schema-based cleaning was introduced only recently [27] in order to reduce the size of automata on nested words. The idea is to remove all rules and states from an automaton that are not used to recognize any word satisfying the schema. Schema-based cleaning can be based on the accessible states of the product of the automaton with the schema. While this product may be larger than the automaton, the schema-based cleaning will always be smaller.

For illustration, the schema-based cleaning of NFA  $\text{det}(A_0)$  in Fig. 3 with respect to schema  $\text{words-one}_{\Sigma}^x$  is given in Fig. 4. The only words recognized by both  $\text{det}(A_0)$  and  $\text{words-one}_{\Sigma}^x$  are  $x$  and  $xa$ . For recognizing these two words, the automaton  $\text{det}(A_0)$  does not need states 2 and 3, so they can be removed with all their transitions rules. Thereby, the word  $xxa$  violating the schema is no more recognized after schema-based cleaning, while it was recognized by  $\text{det}(A_0)$ . Furthermore, note that the state 0 needs no more to be final after schema-based cleaning. Therefore the word  $\varepsilon$ , which is recognized by the automaton but not by the schema, is no more recognized after schema-based cleaning. So schema-based cleaning may change the language of the automaton but only outside of the schema.

Interestingly, the NFA  $A_0$  in Fig. 2 is schema-clean for schema  $\text{words-one}_{\Sigma}^x$  too, even though it is not perfect, in that recognizes the words  $\varepsilon$  and  $xxa$  which are rejected by the schema. The reason is that for recognizing the words  $x$  and  $xa$ , which both satisfy the schema, all 3 states and all 4 transition rules of  $A_0$  are needed. In contrast, we already noticed that the accessible determinization  $\text{det}(A_0)$  in Fig. 3 is not schema-clean for schema  $\text{words-one}_{\Sigma}^x$ . This illustrates that accessible determinization does not always preserve schema-cleanliness. In

$$\frac{q \in I^A \quad s \in I^S}{(q, s) \in I^{A \times S}} \quad \frac{q \in F^A \quad s \in F^S \quad (q, s) \in \mathcal{Q}^{A \times S}}{(q, s) \in F^{A \times S}}$$

$$\frac{q_1 \xrightarrow{a} q_2 \in \Delta^A \quad s_1 \xrightarrow{a} s_2 \in \Delta^S \quad (q_1, s_1) \in \mathcal{Q}^{A \times S}}{(q_1, s_1) \xrightarrow{a} (q_2, s_2) \in \Delta^{A \times S} \quad (q_2, s_2) \in \mathcal{Q}^{A \times S}}$$

Fig. 6: Accessible product  $A \times S = (\Sigma, \mathcal{Q}^{A \times S}, I^{A \times S}, F^{A \times S}, \Delta^{A \times S})$ .

$$\frac{(q, s) \in I^{A \times S}}{q \in I^{\Pi_A(A \times S)}} \quad \frac{(q, s) \in \mathcal{Q}^{A \times S}}{q \in \mathcal{Q}^{\Pi_A(A \times S)}} \quad \frac{(q, s) \in F^{A \times S}}{q \in F^{\Pi_A(A \times S)}} \quad \frac{(q_1, s_1) \xrightarrow{a} (q_2, s_2) \in \Delta^{A \times S}}{q_1 \xrightarrow{a} q_2 \in \Delta^{\Pi_A(A \times S)}}$$

Fig. 7: Projection  $\Pi_A(A \times S) = (\Sigma, \mathcal{Q}^{\Pi_A(A \times S)}, \Delta^{\Pi_A(A \times S)}, I^{\Pi_A(A \times S)}, F^{\Pi_A(A \times S)})$ .

other words, schema-based cleaning may have a stronger cleaning effect after determinization than before.

The schema-based cleaning of an automaton can be defined based on the accessible product of the automaton with the schema. The accessible product  $A \times S$  of two NFAs  $A$  and  $S$  with signature  $\Sigma$  is defined in Fig. 6. This is the usual product, except that only accessible states are admitted. Clearly,  $\mathcal{L}(A \times S) = \mathcal{L}(A) \cap \mathcal{L}(S)$ . Let  $\Pi_A(A \times S)$  be obtained from the accessible product by projecting away the second component, as formally defined in Fig. 7. The schema-based cleaning of  $A$  with respect to schema  $S$  is this projection.

**Definition 3.**  $scl_S(A) = \Pi_A(A \times S)$ .

The fact that  $A \times S$  is restricted to accessible states matches our intuition that all states of  $scl_S(A)$  can be used to read some word in  $\mathcal{L}(A)$  that satisfies schema  $S$ . This can be proven formally under the condition that all states of  $A \times S$  are also co-accessible. Clearly,  $scl_S(A)$  has is obtained from  $A$  by removing states, initial states, final states, and transitions rules. So it is smaller or equal in size  $|scl_S(A)| \leq |A|$  and language  $\mathcal{L}(scl_S(A)) \subseteq \mathcal{L}(A)$ . Still, schema-based cleaning preserves the part of the language within the schema:

**Proposition 4.**  $\mathcal{L}(A) \cap \mathcal{L}(S) = \mathcal{L}(scl_S(A)) \cap \mathcal{L}(S)$ .

Schema-clean deterministic automata may still not be perfect, in that schema-clean DFAs may recognize some words outside the schema. This happens if some state of a DFA is reached both, by a word satisfying the schema and another word that does not satisfy the schema. An example for a DFA that is schema-clean but not perfect for  $words-one\frac{x}{2}$  is given in Fig. 8. It is not perfect since it accepts the non  $V$ -structure  $xaxa$ . The problem is that state 1 can be reached by the words  $a$  and  $xa$ , so one cannot infer from being in state 1 whether some  $x$  was read or not. If one wants to avoid this, one can use the accessible product of the DFA with the schema instead. In the example, this yields the DFA in Fig. 9 that is schema-clean and perfect for  $words-one\frac{x}{2}$ .

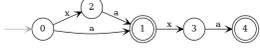


Fig. 8: A DFA that is schema-clean but not perfect for  $words-one_{\Sigma}^x$ .

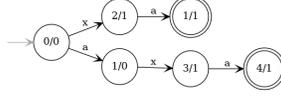


Fig. 9: The accessible product with  $words-one_{\Sigma}^x$  is schema-clean and perfect for  $words-one_{\Sigma}^x$ .

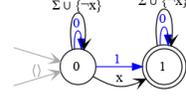


Fig. 10: The  $dSHA$   $one_{\Sigma}^x$  with alphabet  $\Sigma \uplus \{x, \neg x\}$ .

$$\begin{array}{c}
 \frac{Q \in I^{det(A)} \quad I^S = \{s\}}{Q \in I^{det_S(A)} \quad Q \sim s} \quad \frac{Q \sim s}{Q \in Q^{det_S(A)}} \quad \frac{Q \in F^{det(A)} \quad s \in F^S}{Q \in F^{det_S(A)} \quad Q \sim s} \\
 \\
 \frac{Q \xrightarrow{a} Q' \in \Delta^{det(A)} \quad Q \sim s \quad s \xrightarrow{a} s' \in \Delta^S}{Q \xrightarrow{a} Q' \in \Delta^{det_S(A)} \quad Q' \sim s'}
 \end{array}$$

Fig. 11: Schema-based determ.  $det_S(A) = (\Sigma, Q^{det_S(A)}, \Delta^{det_S(A)}, I^{det_S(A)}, F^{det_S(A)})$ .

**Proposition 5.** For any DFAs  $A$  and  $S$  with alphabet  $\Sigma$  the accessible product  $A \times S$  and the schema-based cleaning  $scl_S(A)$  can be computed in expected amortized time  $O(|Q^{A \times S}| |\Sigma| + |A| + |S|)$ .

## 4 Schema-Based Determinization

Schema-based cleaning after determinization becomes impossible in practice if the automaton obtained by determinization is too big. We therefore show next how to integrate schema-based cleaning into automata determinization directly.

The schema-based determinization of  $A$  with respect to schema  $S$  extends on accessible determinization  $det(A)$ . The idea is to run the schema  $S$  in parallel with  $det(A)$ , in order to keep only those state  $Q \in Q^{det(A)}$  that can be aligned to some state  $s \in Q^S$ . In this case we write  $Q \sim s$ .

The schema-determinization  $det_S(A)$  is defined in Fig. 11. The automaton  $det_S(A)$  permits to go from any subset  $Q \in Q^{det(A)}$  and letter  $a \in \Sigma$  to the set of states  $Q' = a^{\Delta^{det(A)}}(Q)$ , under the condition that there exists schema states  $s, s' \in Q^S$  such that  $Q \sim s$  and  $s \xrightarrow{a} s'$ . In this case  $Q' \sim s'$  is inferred.

**Theorem 1 (Correctness).**  $det_S(A) = scl_S(det(A))$  for any NFA  $A$  and DFA  $S$  with the same signature.

The theorem states that schema-based determinization yields the same result that accessible determinization followed by schema-based cleaning.

For preparing the correctness proof we first collapse the two systems of inference rules for accessible products and projection into a single rule system. This yields the rule systems for schema-based cleaning in Fig. 12. The rules there define the automaton  $\widehat{scl}_S(A)$ , that we annotate with a hat, in order to

$$\begin{array}{c}
\frac{q \in I^A \quad s \in I^S}{q \in \widehat{scl}_S(A) \quad (q, s) \in \mathcal{Q}^{A \times S}} \quad \frac{q \in F^A \quad s \in F^S \quad (q, s) \in \mathcal{Q}^{A \times S}}{q \in F^{\widehat{scl}_S(A)}} \\
\frac{(q, s) \in \mathcal{Q}^{A \times S}}{q \in \widehat{scl}_S(A)} \quad \frac{q_1 \xrightarrow{a} q_2 \in \Delta^A \quad s_1 \xrightarrow{a} s_2 \in \Delta^S \quad (q_1, s_1) \in \mathcal{Q}^{A \times S}}{q_1 \xrightarrow{a} q_2 \in \Delta^{\widehat{scl}_S(A)} \quad (q_2, s_2) \in \mathcal{Q}^{A \times S}} \\
\widehat{scl}_S(A) = (\Sigma, \mathcal{Q}^{\widehat{scl}_S(A)}, \Delta^{\widehat{scl}_S(A)}, I^{\widehat{scl}_S(A)}, F^{\widehat{scl}_S(A)})
\end{array}$$

Fig. 12: A collapsed rule systems for schema-based cleaning  $\widehat{scl}_S(A)$ .

distinguish it from the previous automaton  $scl_S(A)$ . The rules also infer judgements  $(q, s) \in \mathcal{Q}^{A \times S}$  that we distinguish by a hat from the previous judgments  $(q, s) \in \mathcal{Q}^{A \times S}$  of the accessible product. The next proposition shows that the system of collapsed inference rules indeed redefines the schema-based cleaning.

**Proposition 6.** *For any two NFAs  $A$  and  $S$  with the same signature:*

$$scl_S(A) = \widehat{scl}_S(A) \quad \text{and} \quad \mathcal{Q}^{A \times S} = \mathcal{Q}^{A \times S}$$

*Proof of Correctness Theorem 1.* Instantiating the system of collapsed rules for schema-based cleaning from Fig. 12 with  $\det(A)$  for  $A$  yields the rule system in Fig. 20. We can identify the instantiated collapsed system for  $\widehat{scl}_S(\det(A))$  with that for  $\det_S(A)$  in Fig. 11, by identifying the judgements  $(Q, s) \in \mathcal{Q}^{\det(A) \times S}$  with judgments  $Q \sim s$ . After renaming the predicates, the inference rules for the corresponding judgments are the same. Hence  $\widehat{scl}_S(\det(A)) = \det_S(A)$ , so that Proposition 6 implies  $scl_S(\det(A)) = \det_S(A)$ .  $\square$

**Proposition 7.** *The schema-based determinization  $\det_S(A)$  for a NFA  $A$  and a DFA  $S$  over  $\Sigma$  can be computed in expected amortized time  $O(|\mathcal{Q}^{\det(A) \times S}| |\Sigma| + |\mathcal{Q}^{\det_S(A)}| |\Delta^A| + |A| + |S|)$ .*

By Proposition 2, computing  $\det(A)$  requires time  $O(|\mathcal{Q}^{\det(A)}| |\Delta^A| + |A|)$ . Therefore, with Proposition 5, the accessible product  $\det(A) \times S$  can be computed from  $A$  and  $S$  in time  $O(|\mathcal{Q}^{\det(A) \times S}| |\Sigma| + |\mathcal{Q}^{\det(A)}| |\Delta^A| + |A| + |S|)$ . Since  $\mathcal{Q}^{\det_S(A)} \subseteq \mathcal{Q}^{\det(A)}$  the proposition shows that schema-based determinization is at most as efficient in the worst case as accessible determinization followed by schema-based cleaning. If  $|\mathcal{Q}^{\det(A) \times S}| |\Sigma| < |\mathcal{Q}^{\det(A)}| |\Delta^A|$  then it is more efficient, since schema-based determinization avoids the computation of  $\det(A)$  all over. Instead, it only computes the accessible product  $\det(A) \times S$ , which may be considerably smaller, since exponentially many states of  $\det(A)$  may not be aligned to any state of  $S$ . Sometimes, however, the accessible product may be bigger. In this case, schema-based determinization may be more costly than pure accessible determinization, not followed by schema-based cleaning.

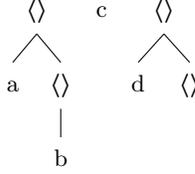
## 5 Stepwise Hedge Automata for Nested Words

We next recall *SHAs* [27] for defining languages of nested words, regular schemas and queries. Nested words generalize on words by adding parenthesis that must

be well-nested. While containing words natively, they also generalize on unranked trees, and hedges. We restrict ourselves to nested words with a single pair of opening and closing parenthesis  $\langle$  and  $\rangle$ . Nested words over a finite alphabet  $\Sigma$  of internal letters have the following abstract syntax.

$$w, w' \in \mathcal{N}_\Sigma ::= \varepsilon \mid a \mid \langle w \rangle \mid w \cdot w' \quad \text{where } a \in \Sigma$$

We assume that concatenation  $\cdot$  is associative and that the empty word  $\varepsilon$  is a neutral element, that is  $w \cdot (w' \cdot w'') = (w \cdot w') \cdot w''$  and  $\varepsilon \cdot w = w = w \cdot \varepsilon$ . Nested words can be identified with hedges, i.e., words of unranked trees and letters from  $\Sigma$ . Seen as a graph, the inner nodes are labeled by the tree constructor  $\langle \rangle$  and the leaves by symbols in  $\Sigma$  or the tree constructor. For instance  $\langle a \cdot \langle b \rangle \cdot \varepsilon \rangle \cdot c \cdot \langle d \cdot \langle \varepsilon \rangle \rangle$  corresponds to the hedge on the right.



A nested word of type *tree* has the form  $\langle h \rangle$ . Note that dangling parentheses are ruled out and that labeled parentheses can be simulated by using internal letters. *XML* documents are labeled unranked trees, for instance:  $\langle a \text{ name} = \text{"uf f"} \rangle \langle b \text{ isgaga} \langle d \rangle \langle b \rangle \langle c \rangle \langle a \rangle$ . Labeled unranked trees satisfying the *XML* data model can be represented as nested words over a signature that contains the *XML* node-types (*elem*, *attr*, *text*, ...), the *XML* names of the document ( $a, \dots, d, \text{name}$ ), and the characters of the data values, say UTF8. For the above example, we get the nested word  $\langle \text{elem} \cdot a \cdot \langle \text{attr} \cdot \text{name} \cdot u \cdot f \cdot f \rangle \langle \text{elem} \cdot b \cdot \langle \text{text} \cdot i \cdot s \cdot g \cdot a \cdot g \cdot a \rangle \langle \text{elem} \cdot d \rangle \rangle \langle \text{elem} \cdot c \rangle$

**Definition 8.** A *SHA* is a tuple  $A = (\Sigma, \mathcal{Q}, \Delta, I, F)$  where  $\Delta = (\Delta', @^\Delta, \diamond^\Delta)$  such that  $(\Sigma, \mathcal{Q}, \Delta', I, F)$  is a NFA,  $\diamond^\Delta \subseteq \mathcal{Q}$  is a set of tree initial states and  $@^\Delta \subseteq \mathcal{Q}^3$  a set of apply rules.

*SHAs* can be drawn as graphs while extending on the graphs of NFAs. A tree initial state  $q \in \diamond^\Delta$  is drawn as a node  $\overset{\langle \rangle}{\rightarrow} q$  with an incoming tree arrow. An applyrule  $(q_1, q, q_2) \in @^\Delta$  is drawn as a blue edge  $\overset{q}{\rightarrow} q_2$  that is labeled by a state  $q \in \mathcal{Q}$  rather than a letter  $a \in \Sigma$ . It states that a nested word in state  $q_1$  can be extended by a tree in state  $q$  and become a nested word in state  $q_2$ .

For instance, the *SHA*  $\text{one}_\Sigma^x$  is drawn graphically in Fig. 10. It accepts all nested words over  $\Sigma \uplus \{x, \neg x\}$  that contain exactly one occurrence of letter  $x$ . Compared to the NFA  $\text{words-one}_{\Sigma \uplus \{\neg x\}}^x$  from Fig. 5, the *SHA*  $\text{one}_\Sigma^x$  contains three additional apply rules  $(0, 0, 0), (0, 1, 1), (1, 0, 1) \in @^{\Delta^{\text{one}_\Sigma^x}}$  for reading the states assigned to subtrees. The state 0 is chosen as the single tree initial state.

Transitions for NFAs on words can be lifted to transitions for *SHAs* of the form  $q \xrightarrow{w} q'$  wrt  $\Delta$  where  $w \in \mathcal{N}_\Sigma$  and  $q, q' \in \mathcal{Q}$ . For this, we add the following inference rule to the previous inference rules for NFAs:

$$\frac{q' \in \diamond^\Delta \quad q' \xrightarrow{w} q \text{ wrt } \Delta \quad (q_1, q, q_2) \in @^\Delta}{q_1 \xrightarrow{\langle w \rangle} q_2 \text{ wrt } \Delta}$$

The rule says that a tree  $\langle w \rangle$  can transit from a state  $q_1$  to a state  $q_2$  if there is an apply rule  $(q_1, q, q_2) \in @^\Delta$  so that  $w$  can transit from some tree initial state

$$\frac{\diamond^{\Delta^A} \neq \emptyset}{\diamond^{\Delta^A} \in \mathcal{Q}^{\det(A)}} \quad \frac{Q_1 \in \mathcal{Q}^{\det(A)} \quad Q_2 \in \mathcal{Q}^{\det(A)} \quad Q' = \{q' \in \mathcal{Q}^A \mid q_1 @ q_2 \rightarrow q' \in \Delta^A, q_1 \in Q_1, q_2 \in Q_2\} \neq \emptyset}{Q_1 @ Q_2 \rightarrow Q' \in \Delta^{\det(A)} \quad Q' \in \mathcal{Q}^{\det(A)}}$$

Fig. 13: Accessible determinization  $\det(A)$  lifted from NFAs to *SHAs*.

$q' \in \diamond^{\Delta}$  to  $q$ . Otherwise, the language  $\mathcal{L}(A)$  of nested words accepted by a *SHA*  $A$  is defined as in the case of NFAs.

**Definition 9.** A *SHA*  $(\Sigma, \mathcal{Q}, \Delta, I, F)$  is deterministic or equivalently a *dSHA*, if it satisfies the following conditions:

- $I$  and  $\diamond^{\Delta}$  both contain at most one element,
- $a^{\Delta}$  is a partial function from  $\mathcal{Q}$  to  $\mathcal{Q}$  for all  $a \in \Sigma$ , and
- $@^{\Delta}$  is a partial function from  $\mathcal{Q} \times \mathcal{Q}$  to  $\mathcal{Q}$ .

Note that if  $A$  is a *dSHA* and  $\Delta = (\Delta', @^{\Delta}, \diamond^{\Delta})$  then  $A' = (\Sigma, \mathcal{Q}, \Delta', I, F)$  is a DFA. Conversely any DFA  $A'$  defines a *dSHA* with  $@^{\Delta} = \emptyset$  and  $I = \emptyset$ . For instance, the *SHA*  $one_{\Sigma}^x$  in Fig. 10 contains the DFA  $words-one_{\Sigma \uplus \{\neg x\}}^x$  from Fig. 5 with  $\Sigma$  instantiated by  $\Sigma \uplus \{x\}$ .

A schema for nested words over  $\Sigma$  is a *dSHA* over  $\Sigma$ . Note that schemas for nested words generalize over schemas of words, since *dSHAs* generalize on DFAs. The rules for the accessible determinization  $\det(A)$  of a *SHA*  $A$  in Fig. 13 extend on those for NFAs in Fig. 1. As for words,  $\det(A)$  is always deterministic, recognizes the same language as  $A$ , and contains only accessible states.

**Proposition 10.** The accessible determinization of a *SHA* can be computed in expected amortized time  $O(|\mathcal{Q}^{\det(A)}|^2 |\Delta^A| + |A|)$ .

The notions of monadic query functions  $\mathbf{Q}$  can be lifted from words to nested words, so that it selects nodes of the graph a nested word. For this, we have to fix one of manner possible manners to define identifiers for these nodes. The set of nodes of a nested word  $w$  is denoted by  $nod(w) \subseteq \mathbb{N}$ .

For indicating the selection of node  $\pi \in nod(w)$ , we insert the variable  $x$  into the sequence of letters following the opening parenthesis of  $\pi$ . If we don't want to select  $\pi$ , we insert the letter  $\neg x$  instead. For any nested word  $w$  with alphabet  $\Sigma$ , the nested word  $w[\pi/x]$  obtained by insertion of  $x$  or  $\neg x$  at a node  $\pi \in nod(w)$  has alphabet  $\Sigma \uplus \{x, \neg x\}$ . As before, we define  $L_{\mathbf{Q}} = \{w*[\pi/x] \mid w \in \mathcal{N}_{\Sigma}, \pi \in \mathbf{Q}(w)\}$ .

The notion of a query automata can now be lifted from words to nested words straightforwardly: a query automaton for nested words over  $\Sigma$  is a *SHA*  $A$  with alphabet  $\Sigma \cup \{x, \neg x\}$ . It defines the unique total query  $\mathbf{Q}$  such that  $L_{\mathbf{Q}} = \mathcal{L}(A) \cap \mathcal{L}(one_{\Sigma}^x)$ . A deterministic query automaton for the XPATH QN7 on XML documents is given in Fig. 14.

## 6 Schema-Based Determinization for SHAs

We can lift all previous algorithms from NFAs to *SHAs* while extending the system of inference rules. The additional rules concern tree initial states, that

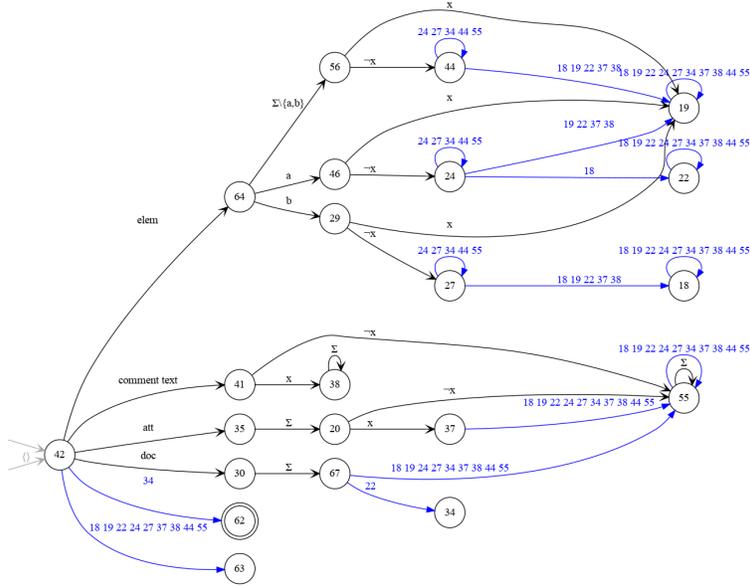


Fig. 14: A  $one_{\Sigma}^x$ -cleaned minimal  $dSHA$  for the XPATH query QN7.

$$\frac{q \in \diamond^{\Delta^A} \quad s \in \diamond^{\Delta^S}}{(q, s) \in \diamond^{\Delta^{A \times S}}} \quad \frac{(q_1, s_1) \in \mathcal{Q}^{A \times S} \quad (q, s) \in \mathcal{Q}^{A \times S}}{(q_1, s_1) @ (q, s) \rightarrow (q_2, s_2) \in \Delta^{A \times S}} \quad \frac{q_1 @ q \rightarrow q_2 \in \Delta^A \quad s_1 @ s \rightarrow s_2 \in \Delta^S}{(q_2, s_2) \in \mathcal{Q}^{A \times S}}$$

Fig. 15: Lifting accessible products to  $SHAs$ .

work in analogy to initial states, and also apply rules that works similarly as internal rules. The new inference rules for accessible products  $A \times S$  are given in Fig. 15 and for projection  $\Pi_A A \times S$  in Fig. 16. As before we define  $scl_S(A) = \Pi_A(A \times S)$ . The rules for schema schema-based determinization  $det_S(A)$  are extended in Fig. 17. The next complexity upper bound, however, now become quadratic with fixed alphabet:

**Proposition 11.** *If  $A$  and  $S$  are  $dSHAs$  then the accessible product  $A \times S$  and the schema-based cleaning  $scl_S(A)$  can be computed in expected amortized time  $O(|\mathcal{Q}^{A \times S}|^2 + |\mathcal{Q}^{A \times S}| |\Sigma| + |A| + |S|)$ .*

**Theorem 2 (Correctness).** *For any  $SHA A$  and  $dSHA S$  with the same alphabet it holds that  $det_S(A) = scl_S(det(A))$ .*

The proof extends on that for NFAs (Theorem 1) in a direct manner.

**Proposition 12.** *The schema-based determinization  $det_S(A)$  of a  $SHA A$  with respect to a  $dSHA S$  can be computed in expected amortized time  $O(|\mathcal{Q}^{det(A) \times S}|^2 + |\mathcal{Q}^{det(A) \times S}| |\Sigma| + |\mathcal{Q}^{det_S(A)}|^2 |\Delta^A| + |A| + |S|)$ .*

$$\frac{(q, s) \in \diamond^{\Delta^{A \times S}}}{q \in \diamond^{\Delta^{\Pi_A(A \times S)}}} \quad \frac{(q_1, s_1) @ (q, s) \rightarrow (q_2, s_2) \in \Delta^{A \times S}}{q_1 @ q \rightarrow q_2 \in \Delta^{\Pi_A(A \times S)}}$$

Fig. 16: Lifting projections  $\Pi_A(A \times S)$  to *SHAs*.

$$\frac{\diamond^{\Delta^S} = \{s\}}{\diamond^{\Delta^A} \in \diamond^{\Delta^{\det_S(A)}} \quad \diamond^{\Delta^A} \sim s} \quad \frac{s_1 @ s_2 \rightarrow s' \in \Delta^S \quad Q_1 \sim s_1 \quad Q_2 \sim s_2}{Q_1 @ Q_2 \rightarrow Q' \in \Delta^{\det(A)}} \\ \frac{Q_1 @ Q_2 \rightarrow Q' \in \Delta^{\det_S(A)} \quad Q' \sim s'}$$

Fig. 17: Extension of schema-based determinization to *SHAs*.

By Propositions 10 and 11, computing  $scl_S(\det(A))$  by schema-based cleaning after accessible determinization needs time in  $O(|\mathcal{Q}^{\det(A) \times S}|^2 + |\mathcal{Q}^{\det(A) \times S}| |\Sigma| + |\mathcal{Q}^{\det(A)}|^2 |\Delta^A| + |A| + |S|)$ . This complexity bound is similar to that of schema-based determinization from Proposition 12. Since  $\mathcal{Q}^{\det_S(A)} \subseteq \mathcal{Q}^{\det(A)}$ , Proposition 12 shows that the worst case time complexity of schema-based determinization is never worse than for schema-based cleaning after determinization.

We implemented our algorithm for schema-based determinization in Scala. A description of our implementation and benchmarking results can be found in [1]. We used symbolic *SHAs*, so any  $\Sigma$ -rule is counted as 1. We applied the algorithm to the *SHA* of **QN7** which has 132 states and size 322. Determinization based on schema  $one_{\Sigma}^x$  and the *XML* model produces a *dSHA* with 74 states and size 277. The minimization of this *dSHA* in the class of *dSHAs* with the same initial and tree initial state (see [26]) yields the *dSHA* in Fig. 14. It has 22 states and size 144. In contrast, accessible determinization without any schema produces a *dSHA* with 10.003 states and size 1.633.790, for which our Datalog implementation of schema-based cleaning runs out of memory. An alternative solution can be obtained by accessible determinization of the product  $sha(\mathbf{QN7}) \times one_{\Sigma}^x$ . This yields a *dSHA* with 74 states and size 269, which can then be schema-cleaned with the *XML* data model and minimized.

## 7 Conclusion and Future Work

We presented the first algorithm for schema-based determinization for NFAs and *SHAs* and proved it to produce the same results as determinization followed by schema-based cleaning but with lower worst case complexity. We gave an example of an *SHA* for a regular XPATH query, for which schema-based determinization produces a *dSHA* of size  $< 300$ , while schema-free determinization produces an *dSHA* of size  $> 1.5$  million. In a subsequent paper [1], we show how our approach can be lifted to symbolic *SHAs* for dealing with large, infinite, and typed alphabets, so that it can be applied successfully to all forwards navigational XPATH queries of the XPath benchmark [22], that Lick and Schmitz extracted from practical XSLT and XQuery programs.

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## A Proofs for Section 1 (Introduction)

### A.1 Further Related Work

**Nested regular path queries.** [21,23] are formulas from propositional dynamic logic (PDL) [15]. While applicable to general data graphs, they can also be restricted to nested words. They extend on usual regular expression by adding nested filters that are closed under the logical operators. Filters may test for the existence of nodes answering a nested regular path query. When XML documents, nested regular path queries can be identified with regular forward XPath queries [5,19].

**MSO.** It is folklore that nested regular path queries on data trees can be compiled to automata. For ranked trees, one can first compile path queries to monadic second-order (MSO) formulas, and from there to tree automata that recognize so-called V-structures [32,18,10]. V-structures are trees that are annotated with variables, saying where the query is going to select a node. In recent database terminology, languages of V-structures are called document spanners [14,29]. But since the compilation of path queries to MSO formulas eagerly introduces quantifier alternations, that are to be eliminated by repeated automata determinization, this approach leads to a large size blowup.

**Nested Regular Expressions.** A more recent idea [7] is to compile nested regular path queries to nested regular expressions in a first step, i.e., regular expressions for nested words that were introduced earlier under the name *regular expression types* by Hosoya and Pierce [20]. Nested regular expressions support the usual operators of regular expressions and the nesting expressions  $\langle e \rangle$  for defining languages of nested words. Furthermore, they support vertically recursive definitions based on  $\mu$ -expressions  $\mu x.e$ , intersections  $e \cap e'$ , and complementation  $\bar{e}$ . It is then possible to compile nested regular expressions to *SHAs* or *NWAs*, by lifting the usual automata constructions from standard regular to nested regular expressions.

**Forest Algebras.** Nested words are very similar to forests, i.e., sequences of ranked trees. The difference is that letters of nested words need to be encoded into single node trees. The transition relation of any *SHA* can be used to define a forest algebra [6].

**Hedge Automata.** In contrast to classical hedge automata [31,11] *SHAs* come with a satisfying notion of determinism.

## B Proofs for Section 2 (Finite Automata on Words, Schemas, and Queries)

*Proof.* An algorithm computing the fixed point of the inference rules for accessible determinization in Fig. 1 is presented in Fig. 18. It uses dynamic perfect hashing [13] for implementing hash sets, so that set inserting and membership can be done in randomized amortized time  $O(1)$ . The algorithm has a hash set *Store* to save all discovered states  $Q^{det(A)}$  and a hash set *Rules* to collect all transition rules. Furthermore, it has a stack *Agenda* to process all new states  $Q \in Q^{det(A)}$ . For each  $Q$  popped from the stack *Agenda*, the algorithm uses

```

1  let Store = hashset.new( $\emptyset$ )
2  let Agenda = list.new() and Rules = hashset.new( $\emptyset$ )
3  if  $init^A \neq \emptyset$  then Agenda.add( $init^A$ )
4  while Agenda.notEmpty() do
5      let Q = Agenda.pop()
6      let h be an empty hashtable with keys from  $\Sigma$ .
7          // the values will be nonempty hash subsets of  $\mathcal{Q}^A$ 
8      for  $q \xrightarrow{a} q' \in \Delta^A$  such that  $q \in Q$  do
9          if h.get(a) = undef then h.add(a, hashset.new( $\emptyset$ ))
10         (h.get(a)).add( $q'$ )
11     for (a,  $Q'$ ) in h.tolist() do Rules.add( $Q \xrightarrow{a} Q'$ )
12     if not Store.member( $Q'$ ) then Store.add( $Q'$ ) Agenda.push( $Q'$ )
    
```

Fig. 18: An algorithm computing the accessible determinization  $\det(A)$  of a NFA  $A$  by applying the inference rules from Fig. 1.

a hashtable  $h$  to compute all pairs  $(a, Q')$  such that  $Q \xrightarrow{a} Q' \in \Delta^{\det(A)}$  and  $Q' \neq \emptyset$ . This is done by iterating of  $\Delta^A$  so in time  $O(|\Delta^A|)$ . By iterating over the hashtable  $h$ , all transitions  $Q \xrightarrow{a} Q'$  will be added to the set  $Rules$  and  $Q'$  will be added to the stack  $Agenda$  and to the hash set  $Store$  if it wasn't there yet. The overall number of elements in the  $Agenda$  is  $|\mathcal{Q}^{\det(A)}|$ . For each  $Q$ , the computation of all  $Q'$  is in time  $O(|\Delta^A|)$ . The preprocessing of  $A$  requires time  $O(|A|)$ . Thus, the total time of the algorithm is in  $O(|\mathcal{Q}^{\det(A)}| |\Delta^A| + |A|)$ .  $\square$

### C Proofs for Section 3 (Schema-Based Cleaning)

**Proposition 5.** *For any DFAs  $A$  and  $S$  with alphabet  $\Sigma$  the accessible product  $A \times S$  and the schema-based cleaning  $scl_S(A)$  can be computed in expected amortized time  $O(|\mathcal{Q}^{A \times S}| |\Sigma| + |A| + |S|)$ .*

*Proof.* It is sufficient to show that the accessible product  $A \times S$  can be computed in this time. An algorithm to compute the fixed points of the inference rules for the accessible product  $A \times S$  in Fig. 6 can be organized such that only accessible states are considered (similarly to semi-naive datalog evaluation). This algorithm is presented in Fig. 19. It dynamically generates the set of rules  $Rules$  by using perfect dynamic hashing [13]. Testing set membership is in time  $O(1)$  and the addition of elements to the set is in expected amortized time  $O(1)$ . The algorithm uses a stack,  $Agenda$ , to memoize all new pairs  $(q_1, s_1) \in \mathcal{Q}^{A \times S}$  that need to be preprocessed, and a hash set  $Store$  that saves all processed states  $\mathcal{Q}^{A \times S}$ . We aim not to push the same pair more than once in the  $Agenda$ . For this, membership to the  $Store$  is checked before an element is pushed to the  $Agenda$ . For each pair popped from the stack  $Agenda$ , the algorithm does the following: for each letter  $a \in \Sigma$  it computes the sets  $Q = \{q_2 \mid q_1 \xrightarrow{a} q_2 \in \Delta^A\}$  and  $R = \{s_2 \mid s_1 \xrightarrow{a} s_2 \in \Delta^S\}$  and then adds the subset of states of  $Q \times R$  that were not stored in the hash set  $Store$  to the agenda. Since  $A$  and  $S$  are deterministic, there is at most one such pair, so the time for treating one pair on the agenda is in expected

```

1 if  $init^A = \{q_0\}$  and  $init^S = \{s_0\}$  then  $Agenda.add((q_0, s_0))$ 
2 while  $Agenda.notEmpty()$  do
3   let  $(q_1, s_1) = Agenda.pop()$ 
4   for  $a \in \Sigma$  do
5     let  $Q = \{q_2 \mid q_1 \xrightarrow{a} q_2 \in \Delta^A\}$   $R = \{s_2 \mid s_1 \xrightarrow{a} s_2 \in \Delta^S\}$ 
6     for  $q_2 \in Q$  and  $s_2 \in R$  do
7        $Rules.add((q_1, s_1) \xrightarrow{a} (q_2, s_2))$ 
8       if not  $Store.member((q_2, s_2))$ 
9         then  $Store.add((q_2, s_2))$   $Agenda.push((q_2, s_2))$ 

```

Fig. 19: An algorithm computing the fixed point of the inference rules of the accessible product of DFAs  $A$  and  $S$ , using a stack  $Agenda$ , a hash set  $Store$  for the states, and a hash set  $Rules$  for the transition rules.

amortized time  $O(|\Sigma|)$ . The overall number of elements in the agenda will be  $|\mathcal{Q}^{A \times S}|$ . Note that  $Q$  and  $R$  can be computed in  $O(1)$  after preprocessing  $A$  and  $S$  in time  $O(|A| + |S|)$ . Therefore, we will have a total time of the algorithm in  $O(|\mathcal{Q}^{A \times S}| |\Sigma| + |A| + |S|)$ .  $\square$

## D Proofs for Section 4 (Schema-Based Determinization)

**Proposition 6.** *For any two NFAs  $A$  and  $S$  with the same signature:*

$$scl_S(A) = \widehat{scl}_S(A) \quad \text{and} \quad \mathcal{Q}^{A \times S} = \mathcal{Q}^{A \widehat{\times} S}$$

*Proof.* The two equations are shown by the following four lemmas. The judgments with a hat there are to be inferred by the collapsed system of inference rules in Fig. 12, while the other judgments are to be inferred with the rule system for accessible products in Fig. 6.

**Lemma 13.**  $q \in I^{\widehat{scl}_S(A)}$  iff  $q \in I^{scl_S(A)}$ .

*Proof.* The rule systems of accessible product, projection, and the collapsed system can be used as following :

$$\frac{q \in I^A \quad s \in I^S}{q \in I^{\widehat{scl}_S(A)}} \quad \frac{\frac{q \in I^A \quad s \in I^S}{(q, s) \in I^{A \times S}}}{q \in I^{scl_S(A)}}$$

**Lemma 14.**  $(q, s) \in \mathcal{Q}^{A \widehat{\times} S}$  iff  $(q, s) \in \mathcal{Q}^{A \times S}$ .

*Proof.* We proof for all  $n \geq 0$  that if  $(q, s) \in \mathcal{Q}^{A \widehat{\times} S}$  has a proof tree of size  $n$  then there exists a proof tree for  $(q, s) \in \mathcal{Q}^{A \times S}$ . The proof is by induction on  $n$ .

In the case of the rules of the initial states,  $(q, s) \in \mathcal{Q}^{A \widehat{\times} S}$  is inferred directly whenever  $(q, s) \in \mathcal{Q}^{A \times S}$  and vice versa, using the following:

$$\frac{q \in I^A \quad s \in I^S}{(q, s) \in I^{A \times S}} \quad \frac{q \in I^A \quad s \in I^S}{(q, s) \in \mathcal{Q}^{A \times S}} \quad \frac{q \in I^A \quad s \in I^S}{q \in I^{\widehat{scl}_S(A)} \quad (q, s) \in \mathcal{Q}^{A \widehat{\times} S}}$$

If  $(q, s) \in \mathcal{Q}^{A\widehat{\times}S}$  is inferred by the internal rule of the collapsed rule system in Fig. 12. Then the proof tree has the following form for some proof tree  $T_1$ :

$$\frac{q_1 \xrightarrow{a} q_2 \in \Delta^A \quad s_1 \xrightarrow{a} s_2 \in \Delta^S \quad \frac{T_1}{(q_1, s_1) \in \mathcal{Q}^{A\widehat{\times}S}}}{(q_2, s_2) \in \mathcal{Q}^{A\widehat{\times}S}}$$

This shows that there is a smaller proof tree  $T_1$  for inferring  $(q_1, s_1) \in \mathcal{Q}^{A\widehat{\times}S}$ . So by induction hypothesis applied to  $T_1$ , there exists a proof tree  $T'_1$  for inferring  $(q_1, s_1) \in \mathcal{Q}^{A \times S}$  with the proof system of accessible products in Fig. 6:

$$\frac{T'_1}{(q_1, s_1) \in \mathcal{Q}^{A \times S}}$$

Therefore, we also have the following proof tree for  $(q_2, s_2) \in \mathcal{Q}^{A \times S}$  with the internal rule for the accessible product:

$$\frac{q_1 \xrightarrow{a} q_2 \in \Delta^A \quad s_1 \xrightarrow{a} s_2 \in \Delta^S \quad \frac{T'_1}{(q_1, s_1) \in \mathcal{Q}^{A \times S}}}{(q_2, s_2) \in \mathcal{Q}^{A \times S}}$$

For the inverse direction, if  $(q, s) \in \mathcal{Q}^{A \times S}$  is inferred by the internal rule of the accessible product rule system in Fig. 6. Then the proof tree has the following form for some proof tree  $T_1$ :

$$\frac{q_1 \xrightarrow{a} q_2 \in \Delta^A \quad s_1 \xrightarrow{a} s_2 \in \Delta^S \quad \frac{T_1}{(q_1, s_1) \in \mathcal{Q}^{A \times S}}}{(q_2, s_2) \in \mathcal{Q}^{A \times S}}$$

This means that there is a smaller proof tree  $T_1$  for inferring  $(q_1, s_1) \in \mathcal{Q}^{A \times S}$ . By induction hypothesis applied to  $T_1$ , there exists a proof tree  $T'_1$  for inferring  $(q_1, s_1) \in \mathcal{Q}^{A\widehat{\times}S}$  with the collapsed system in Fig. 12:

$$\frac{T'_1}{(q_1, s_1) \in \mathcal{Q}^{A\widehat{\times}S}}$$

which leads to the following proof tree for  $(q_2, s_2) \in \mathcal{Q}^{A \times S}$  with the internal rule for the collapsed system:

$$\frac{q_1 \xrightarrow{a} q_2 \in \Delta^A \quad s_1 \xrightarrow{a} s_2 \in \Delta^S \quad \frac{T'_1}{(q_1, s_1) \in \mathcal{Q}^{A\widehat{\times}S}}}{(q_2, s_2) \in \mathcal{Q}^{A\widehat{\times}S}}$$

**Lemma 15.**  $q_1 \xrightarrow{a} q_2 \in \Delta^{\widehat{scl}_S(A)}$  iff  $q_1 \xrightarrow{a} q_2 \in \Delta^{scl_S(A)}$ .

*Proof.* We prove for all  $n \geq 0$  that, if  $q_1 \xrightarrow{a} q_2 \in \Delta^{\widehat{scl}_S(A)}$  has a proof tree of size  $n$ , then there exists a proof tree for  $q_1 \xrightarrow{a} q_2 \in \Delta^{scl_S(A)}$  and vice versa. The proof

is by induction on  $n$ .

If  $q_1 \xrightarrow{a} q_2 \in \Delta^{\widehat{scl}_S(A)}$  is inferred by the internal rule of the collapsed system, the proof tree will have the following for some tree  $T_1$ :

$$\frac{q_1 \xrightarrow{a} q_2 \in \Delta^A \quad s_1 \xrightarrow{a} s_2 \in \Delta^S \quad \frac{T_1}{(q_1, s_1) \in \mathcal{Q}^{A \times S}}}{q_1 \xrightarrow{a} q_2 \in \Delta^{\widehat{scl}_S(A)}}$$

By Lemma 14 and the rule of internal rules of the accessible product rule system:

$$\frac{q_1 \xrightarrow{a} q_2 \in \Delta^A \quad s_1 \xrightarrow{a} s_2 \in \Delta^S \quad \frac{T'_1}{(q_1, s_1) \in \mathcal{Q}^{A \times S}}}{(q_1, s_1) \xrightarrow{a} (q_2, s_2) \in \Delta^{A \times S}}$$

For the inverse direction, if  $q_1 \xrightarrow{a} q_2 \in \Delta^{scl_S(A)}$  is inferred by the internal rule of the accessible product, the proof tree will have the following for some tree  $T_1$ :

$$\frac{q_1 \xrightarrow{a} q_2 \in \Delta^A \quad s_1 \xrightarrow{a} s_2 \in \Delta^S \quad \frac{T_1}{(q_1, s_1) \in \mathcal{Q}^{A \times S}}}{\frac{(q_1, s_1) \xrightarrow{a} (q_2, s_2) \in \Delta^{A \times S}}{q_1 \xrightarrow{a} q_2 \in \Delta^{scl_S(A)}}$$

By lemma 14 and the rule of internal rules of the collapsed system:

$$\frac{q_1 \xrightarrow{a} q_2 \in \Delta^A \quad s_1 \xrightarrow{a} s_2 \in \Delta^S \quad \frac{T'_1}{(q_1, s_1) \in \mathcal{Q}^{A \times S}}}{q_1 \xrightarrow{a} q_2 \in \Delta^{\widehat{scl}_S(A)}}$$

**Lemma 16.**  $q \in \mathcal{Q}^{\widehat{scl}_S(A)}$  iff  $q \in \mathcal{Q}^{scl_S(A)}$  and  $q \in F^{\widehat{scl}_S(A)}$  iff  $q \in F^{scl_S(A)}$ .

*Proof.* We start proving  $q \in \mathcal{Q}^{\widehat{scl}_S(A)}$  iff  $q \in \mathcal{Q}^{scl_S(A)}$ . By Lemma 14, and rules of construction of the accessible product, projection, and collapsed systems, this lemma holds for some proof trees  $T$  and  $T'$  as follows:

$$\frac{\frac{T}{(q, s) \in \mathcal{Q}^{A \times S}}}{q \in \mathcal{Q}^{scl_S(A)}} \quad \frac{T'}{q \in \mathcal{Q}^{\widehat{scl}_S(A)}}$$

Finally, we show  $q \in F^{\widehat{scl}_S(A)}$  iff  $q \in F^{scl_S(A)}$ . Using Lemma 14, there exists some proof trees  $T$  and  $T'$  that infers  $(q, s) \in \mathcal{Q}^{A \times S}$  and  $(q, s) \in \mathcal{Q}^{A \times S}$  in both ways and therefore having the following form of rules:

$$\frac{q \in F^A \quad s \in F^S \quad \frac{T}{(q, s) \in \mathcal{Q}^{A \times S}}}{q \in F^{\widehat{scl}_S(A)}} \quad \frac{q \in F^A \quad s \in F^S \quad \frac{T'}{(q, s) \in \mathcal{Q}^{A \times S}}}{(q, s) \in F^{A \times S}} \quad \frac{(q, s) \in F^{A \times S}}{q \in F^{scl_S(A)}}$$

$$\begin{array}{c}
 \frac{Q \in I^{\det(A)} \quad s \in I^S}{Q \in I^{\widehat{scl}_S(\det(A))} \quad (Q, s) \in \mathcal{Q}^{\det(A) \times S}} \quad \frac{Q \in F^{\det(A)} \quad s \in F^S \quad (Q, s) \in \mathcal{Q}^{\det(A) \times S}}{Q \in F^{\widehat{scl}_S(\det(A))}} \\
 \frac{(Q, s) \in \mathcal{Q}^{\det(A) \times S}}{Q \in \mathcal{Q}^{\widehat{scl}_S(\det(A))}} \quad \frac{Q_1 \xrightarrow{a} Q_2 \in \Delta^{\det(A)} \quad s_1 \xrightarrow{a} s_2 \in \Delta^S \quad (Q_1, s_1) \in \mathcal{Q}^{\det(A) \times S}}{Q_1 \xrightarrow{a} Q_2 \in \Delta^{\widehat{scl}_S(\det(A))} \quad (Q_2, s_2) \in \mathcal{Q}^{\det(A) \times S}} \\
 \widehat{scl}_S(\det(A)) = (\Sigma, \mathcal{Q}^{\widehat{scl}_S(\det(A))}, \Delta^{\widehat{scl}_S(\det(A))}, I^{\widehat{scl}_S(\det(A))}, F^{\widehat{scl}_S(\det(A))})
 \end{array}$$

Fig. 20: Instantiation of the collapsed rule system for schema-based cleaning from Fig. 12 with  $\det(A)$ .

```

1  if  $init^A \neq \emptyset$  and  $init^S = \{s_0\}$  then  $Agenda.add(init^A \sim s_0)$ 
2  while  $Agenda.notEmpty()$  do
3    let  $(Q_1 \sim s_1) = Agenda.pop()$ 
4    for  $a \in \Sigma$  do
5      let  $P = \{Q_2 \mid Q_1 \xrightarrow{a} Q_2 \in \Delta^{\det(A)}\}$  and  $R = \{s_2 \mid s_1 \xrightarrow{a} s_2 \in \Delta^S\}$ 
6      for  $Q_2 \in P$  and  $s_2 \in R$  do  $Rules.add(Q_1 \xrightarrow{a} Q_2)$ 
7      if not  $Store.member(Q_2 \sim s_2)$ 
8      then  $Store.add(Q_2 \sim s_2)$   $Agenda.push(Q_2 \sim s_2)$ 
    
```

Fig. 21: An algorithm for schema-based NFA determinisation  $det_S(A)$ .

**Proposition 7.** *The schema-based determinization  $det_S(A)$  for a NFA  $A$  and a DFA  $S$  over  $\Sigma$  can be computed in expected amortized time  $O(|\mathcal{Q}^{\det(A) \times S}| |\Sigma| + |\mathcal{Q}^{det_S(A)}| |\Delta^A| + |A| + |S|)$ .*

*Proof.* An algorithm computing the fixed points of the inference rules of schema-based determinization from Fig. 11 is given in Fig. 21. It refines the algorithm computing the accessible product with on-the-fly determinization and projection.

On the stack *Agenda*, the algorithm stores alignments  $Q \sim s$  such that  $(Q, s) \in \mathcal{Q}^{\det(A) \times S}$  that were not considered before. Transition rules of  $det_S(A)$  are collected in hash set *Rules*, using the dynamic perfect hashing aforementioned. The alignments  $Q_1 \sim s_1$  popped from the agenda are processed as follows: For any letter  $a \in \Sigma$ , the sets  $R = \{Q_2 \mid Q_1 \xrightarrow{a} Q_2 \in \Delta^{\det(A)}\}$  and  $P = \{s_2 \mid s_1 \xrightarrow{a} s_2 \in \Delta^S\}$  are computed. One then pushes all new pairs  $Q_2 \sim s_2$  with  $Q_2 \in P$  and  $s_2 \in R$  into the agenda, and adds  $Q_1 \xrightarrow{a} Q_2$  to the set *Rules*. Since  $S$  and  $\det(A)$  are deterministic there is at most one pair  $(Q, s) \in P \times R$  for  $Q_1$  and  $s_1$ . So the time for treating one pair on the agenda is in  $O(|\Sigma|)$  plus the time for building the needed transition rules of  $\det(A)$  from  $\Delta^A$  on the fly. The time for the one the fly computation of transition rules of  $\det(A)$  is in time  $O(|\mathcal{Q}^{det_S(A)}| |\Delta^A|)$ . The overall number of pairs on the agenda is at most  $|\mathcal{Q}^{\det(A) \times S}|$  so the main while loop of the algorithm requires time in  $O(|\mathcal{Q}^{\det(A) \times S}| |\Sigma|)$  apart from on the fly determinization. This will give us an overall complexity for the algorithm in  $O(|\mathcal{Q}^{\det(A) \times S}| |\Sigma| + |\mathcal{Q}^{det_S(A)}| |\Delta^A| + |A| + |S|)$ , with consideration of the preprocessing time of  $A$  and  $S$ .  $\square$

```

1 let Store = hashset.new( $\emptyset$ )
2 let Agenda = list.new() and Rules = hashset.new( $\emptyset$ )
3 if  $init^A \neq \emptyset$  then Agenda.add( $init^A$ )
4 while Agenda.notEmpty() do
5   let (Q) = Agenda.pop()
6   let h be an empty hashtable with keys from  $\Sigma$ .
7   // the values will be nonempty hash subsets of  $\mathcal{Q}^A$ 
8   for  $q \xrightarrow{a} q' \in \Delta^A$  such that  $q \in Q$  do
9     if h.get(a) = undef then h.add(a, hashset.new( $\emptyset$ ))
10    (h.get(a)).add( $q'$ )
11  for (a, Q') in h.toList() do Rules.add(Q  $\xrightarrow{a}$  Q')
12  if not Store.member(Q') then Store.add(Q') Agenda.push(Q')
13  for  $Q_1 \in Store$  do
14    let  $Q' = \{q' \mid q @_{q_1} \rightarrow q', q_1 \in Q_1, q \in Q\}$ 
15    if  $Q' \neq \emptyset$  then Rules.add(Q @  $Q_1 \rightarrow Q'$ )
16    if not Store.member(Q') then Store.add(Q')
17    Agenda.push(Q')
18  let  $Q'' = \{q'' \mid q_1 @ q \rightarrow q'', q_1 \in Q_1, q \in Q\}$ 
19  if  $Q'' \neq \emptyset$  then Rules.add(Q_1 @ Q  $\rightarrow Q''$ )
    if not Store.member(Q'') then Store.add(Q'')
    Agenda.push(Q'')

```

Fig. 22: An algorithm for accessible determinization of SHAs.

## E Proofs for Section 5 (Stepwise Hedge Automata for Nested Words)

**Proposition 10.** *The accessible determinization of a SHA can be computed in expected amortized time  $O(|\mathcal{Q}^{\det(A)}|^2 |\Delta^A| + |A|)$ .*

*Proof.* An algorithm for computing the fixed points of the inference rules of accessible determinization of a SHA is presented in Fig. 22. It extends on the case of NFAs with the same data structures. It uses dynamic perfect hashing for the hash sets. The additional treatment of apply rules, that dominates the complexity of the algorithm, works as follows: for each  $Q \in \mathcal{Q}^{\det(A)}$  in the *Agenda* and each state  $Q_1 \in \mathcal{Q}^{\det(A)}$  in the *Store*, it computes the sets  $Q' = \{q' \mid q @_{q_1} \rightarrow q', q_1 \in Q_1, q \in Q\}$  and  $Q'' = \{q'' \mid q_1 @ q \rightarrow q'', q_1 \in Q_1, q \in Q\}$  and puts all new non-empty sets in both the *Agenda* and the *Store*, while adding dynamically the generated apply rules in the hash set *Rules*. Again, the overall number of elements in the agenda will be  $|\mathcal{Q}^{\det(A)}|$ , requiring time in  $O(|\mathcal{Q}^{\det(A)}|^2 |\Delta^A|)$ . With a precomputation time of  $A$  in  $O(|A|)$ , the total computation will be in  $O(|\mathcal{Q}^{\det(A)}|^2 |\Delta^A| + |A|)$ .  $\square$

```

1  if  $init^A = \{q_0\}$  and  $init^S = \{s_0\}$  then  $Agenda.add((q_0, s_0))$ 
2  while  $Agenda.notEmpty()$  do
3      let  $(q_1, s_1) = Agenda.pop()$ 
4      for  $a \in \Sigma$  do
5          let  $Q = \{q_2 \mid q_1 \xrightarrow{a} q_2 \in \Delta^A\}$  and  $R = \{s_2 \mid s_1 \xrightarrow{a} s_2 \in \Delta^S\}$ 
6          for  $q_2 \in Q$  and  $s_2 \in R$  do  $Rules.add((q_1, s_1) \xrightarrow{a} (q_2, s_2))$ 
7              if not  $Store.member((q_2, s_2))$ 
8                  then  $Store.add((q_2, s_2))$   $Agenda.push((q_2, s_2))$ 
9          for  $(q, s) \in Store$  do
10             let  $Q' = \{q_2 \mid q_1 @ q \rightarrow q_2 \in \Delta^A\}$  and  $R' = \{s_2 \mid s_1 @ s \rightarrow s_2 \in \Delta^S\}$ 
11             for  $q_2 \in Q'$  and  $s_2 \in R'$  do  $Rules.add((q_1, s_1) \xrightarrow{(q,s)} (q_2, s_2))$ 
12                 if not  $Store.member((q_2, s_2))$ 
13                     then  $Store.add((q_2, s_2))$   $Agenda.push((q_2, s_2))$ 
14             let  $Q'' = \{q_2 \mid q @ q_1 \rightarrow q_2 \in \Delta^A\}$  and  $R'' = \{s_2 \mid s @ s_1 \rightarrow s_2 \in \Delta^S\}$ 
15             for  $q_2 \in Q''$  and  $s_2 \in R''$  do  $Rules.add((q, s) \xrightarrow{(q_1,s_1)} (q_2, s_2))$ 
16                 if not  $Store.member((q_2, s_2))$ 
17                     then  $Store.add((q_2, s_2))$   $Agenda.push((q_2, s_2))$ 
    
```

Fig. 23: An algorithm computing the fixed point of the inference rules the accessible product of  $dSHAs$   $A$  and  $S$ , using a stack  $Agenda$ , a hash set  $Store$  for the states, and a hash set for the transition rules.

## F Proofs for Section 6 (Schema-Based Determinization for SHAs)

**Proposition 11.** *If  $A$  and  $S$  are  $dSHAs$  then the accessible product  $A \times S$  and the schema-based cleaning  $scl_S(A)$  can be computed in expected amortized time  $O(|\mathcal{Q}^{A \times S}|^2 + |\mathcal{Q}^{A \times S}| |\Sigma| + |A| + |S|)$ .*

*Proof.* The algorithm in Fig. 23 is obtained by lifting the algorithm for DFAs in Fig. 19 to  $SHAs$ . For the case of apply rules, we have to combine each pair  $(q_1, s_1) \in \mathcal{Q}^{A \times S}$  in the stack  $Agenda$  with all  $(q, s) \in \mathcal{Q}^{A \times S}$  in the hash set  $Store$ , in both directions. The time to treat these pairs is  $O(|\mathcal{Q}^{A \times S}|^2)$ , so quadratic in the worst case. As before, no state  $(q_1, s_1)$  will be processed twice, due to the set membership test before pushing a pair into the agenda.  $\square$

**Proposition 12.** *The schema-based determinization  $det_S(A)$  of a  $SHA$   $A$  with respect to a  $dSHA$   $S$  can be computed in expected amortized time  $O(|\mathcal{Q}^{det(A) \times S}|^2 + |\mathcal{Q}^{det(A) \times S}| |\Sigma| + |\mathcal{Q}^{det_S(A)}|^2 |\Delta^A| + |A| + |S|)$ .*

*Proof.* Analogous to the case of NFAs on words. The algorithm in Fig. 24 computes the fixed point of the inference rules of schema-based determinization of  $SHAs$ . As for NFAs, it stores untreated alignments on a stack  $Agenda$  and processed alignments in a hash set  $Store$ . It also collects transition rules in a hash set  $Rules$ . New alignments can now be produced by the the inference rule for apply transitions: for each alignment  $Q_1 \sim s_1$  on the  $Agenda$  and  $Q_2 \sim s_2$

```

1  if  $init^A \neq \emptyset$  and  $init^S = \{s_0\}$  then  $Agenda.add(init^A \sim s_0)$ 
2  while  $Agenda.notEmpty()$  do
3    let  $(Q_1 \sim s_1) = Agenda.pop()$ 
4    for  $a \in \Sigma$  do
5      let  $P = \{Q_2 \mid Q_1 \xrightarrow{a} Q_2 \in \Delta^{det(A)}\}$  and  $R = \{s_2 \mid s_1 \xrightarrow{a} s_2 \in \Delta^S\}$ 
6      for  $Q_2 \in P$  and  $s_2 \in R$  do  $Rules.add(Q_1 \xrightarrow{a} Q_2)$ 
7        if not  $Store.member(Q_2 \sim s_2)$ 
8          then  $Store.add(Q_2 \sim s_2)$   $Agenda.push(Q_2 \sim s_2)$ 
9    for  $(Q \sim s) \in Store$  do
10     let  $P' = \{Q_2 \mid Q_1 @ Q \rightarrow Q_2 \in \Delta^{det(A)}\}$  and  $R' = \{s_2 \mid s_1 @ s \rightarrow s_2 \in \Delta^S\}$ 
11     for  $Q_2 \in P'$  and  $s_2 \in R'$  do  $Rules.add(Q_1 @ Q \rightarrow Q_2)$ 
12       if not  $Store.member(Q_2 \sim s_2)$ 
13         then  $Store.add(Q_2 \sim s_2)$   $Agenda.push(Q_2 \sim s_2)$ 
14     let  $P'' = \{Q_2 \mid Q @ Q_1 \rightarrow Q_2 \in \Delta^{det(A)}\}$  and  $R'' = \{s_2 \mid s @ s_1 \rightarrow s_2 \in \Delta^S\}$ 
15     for  $Q_2 \in P''$  and  $s_2 \in R''$  do  $Rules.add(Q @ Q_1 \rightarrow Q_2)$ 
16       if not  $Store.member(Q_2 \sim s_2)$ 
17         then  $Store.add(Q_2 \sim s_2)$   $Agenda.push(Q_2 \sim s_2)$ 

```

Fig. 24: An algorithm for schema-based determinization of *SHAs*

$$\frac{q \in \Diamond^{\Delta^A} \quad s \in \Diamond^{\Delta^S}}{q \in \Diamond^{\Delta^{scl_S(A)}} \quad (q, s) \in \mathcal{Q}^{A \hat{\times} S}}$$

$$\frac{q_1 @ q \rightarrow q_2 \in \Delta^A \quad s_1 @ s \rightarrow s_2 \in \Delta^S \quad (q_1, s_1) \in \mathcal{Q}^{A \hat{\times} S} \quad (q, s) \in \mathcal{Q}^{A \hat{\times} S}}{q_1 @ q \rightarrow q_2 \in \Delta^{scl_S(A)} \quad (q_2, s_2) \in \mathcal{Q}^{A \hat{\times} S}}$$

Fig. 25: Lifting the collapsed rule system from NFAs to *SHAs*.

in the *Store*, the algorithm computes the sets  $\{s \mid s_1 @ s_2 \rightarrow s \in \Delta^S\}$  and  $\{Q \mid Q_1 @ Q_2 \rightarrow Q \in \Delta^{det(A)}\}$  and the to push all pairs  $Q \sim s$  outside the *Store* to the *Agenda*. There may be at most one such pair since  $S$  and  $det(A)$  are deterministic. We also have to consider the symmetric case where  $Q_1 \sim s_1$  on the store and  $Q_2 \sim s_2$  on the *Agenda*. Thus, it is in time  $O(|\mathcal{Q}^{det(A) \times S}|^2)$  which is quadratic in the worst case. Added to the latter, the cost of computing the transition of  $det(A)$  on the fly which is in worst case  $O(|\mathcal{Q}^{det_S(A)}|^2 |\Delta^A| + |A|)$ . Therefore, having the whole algorithm running, including the time for computing the internal rules, in  $O(|\mathcal{Q}^{det(A) \times S}|^2 + |\mathcal{Q}^{det(A) \times S}| |\Sigma| + |\mathcal{Q}^{det_S(A)}|^2 |\Delta^A| + |A| + |S|)$ .  $\square$

## G Proof of Correctness Theorem 2

The proof extends on the proof of the case of words (Theorem 1) in a direct manner.

We first lift the collapsed rule system for NFAs from Fig. 12 to *SHAs* in Fig. 25, and then show that collapsed rules also redefine the schema-based cleaning  $\widehat{scl}_S(A) = scl_S(A)$  in the case of *SHAs*.

**Proposition 17.** *For any two SHAs  $A$  and  $S$  with the same signature:*

$$\Pi_A(A \times S) = \widehat{scl}_S(A) \quad \text{and} \quad \mathcal{Q}^{A \times S} = \mathcal{Q}^{A \widehat{\times} S}$$

*Proof.* The two equations are shown either by new lemmas or an extension of the lemmas from the proof of Theorem 1, whereas all unchanged existing lemmas hold (Lemmas 13, 15 and 16).

**Lemma 18.**  $q \in \langle \rangle^{\Delta^{\widehat{scl}_S(A)}} \text{ iff } \langle \rangle^{\Delta^{scl_S(A)}}$

*Proof.* The rule systems of accessible product, projection and the collapsed system can be used as following :

$$\frac{q \in \langle \rangle^{\Delta^A} \quad s \in \langle \rangle^{\Delta^S}}{q \in \langle \rangle^{\Delta^{\widehat{scl}_S(A)}}} \qquad \frac{q \in \langle \rangle^{\Delta^A} \quad s \in \langle \rangle^{\Delta^S}}{(q, s) \in \langle \rangle^{\Delta^{A \times S}}} \qquad \frac{(q, s) \in \langle \rangle^{\Delta^{A \times S}}}{q \in \langle \rangle^{\Delta^{scl_S(A)}}$$

**Lemma 19 (extends Lemma 14).**  $(q, s) \in \mathcal{Q}^{A \widehat{\times} S} \text{ iff } (q, s) \in \mathcal{Q}^{A \times S}.$

All proofs for initial states rules and internal rules from the previous lemma hold and we extend it for tree initial rules and apply rules:

*Proof.* Similarly, we prove for all  $n \geq 0$  that if  $(q, s) \in \mathcal{Q}^{A \widehat{\times} S}$  has a proof tree of size  $n$  then there exists a proof trees for  $(q, s) \in \mathcal{Q}^{A \times S}$ . The proof is by induction on  $n$ .

In the case of tree initial rules,  $(q, s) \in \mathcal{Q}^{A \widehat{\times} S}$  is inferred directly whenever  $(q, s) \in \mathcal{Q}^{A \times S}$  and vice versa, using the following:

$$\frac{q \in \langle \rangle^{\Delta^A} \quad s \in \langle \rangle^{\Delta^S}}{(q, s) \in \langle \rangle^{\Delta^{A \times S}}} \qquad \frac{q \in \langle \rangle^{\Delta^A} \quad s \in \langle \rangle^{\Delta^S}}{q \in \langle \rangle^{\widehat{scl}_S(A)} \quad (q, s) \in \mathcal{Q}^{A \widehat{\times} S}}$$

In the same spirit, if  $(q, s) \in \mathcal{Q}^{A \widehat{\times} S}$  is inferred by the apply rule of the same system, then the proof tree has the following form for some proof trees  $T_1$  and  $T$ :

$$\frac{q_1 @ q \rightarrow q_2 \in \Delta^A \quad s_1 @ s \rightarrow s_2 \in \Delta^S \quad \frac{T_1}{(q_1, s_1) \in \mathcal{Q}^{A \widehat{\times} S}} \quad \frac{T}{(q, s) \in \mathcal{Q}^{A \widehat{\times} S}}}{(q_2, s_2) \in \mathcal{Q}^{A \widehat{\times} S}}$$

This means that there are smaller proof trees  $T_1$  and  $T$  for inferring respectively  $(q_1, s_1) \in \mathcal{Q}^{A \widehat{\times} S}$  and  $(q, s) \in \mathcal{Q}^{A \widehat{\times} S}$ . Correspondingly, by induction hypothesis applied to  $T_1$  and  $T$ , there exists  $T'_1, T'$  for inferring  $(q_1, s_1) \in \mathcal{Q}^{A \times S}$  and  $(q, s) \in \mathcal{Q}^{A \times S}$ :

$$\frac{T'_1}{(q_1, s_1) \in \mathcal{Q}^{A \times S}} \qquad \frac{T'}{(q, s) \in \mathcal{Q}^{A \times S}}$$

Thus allowing the following proof tree for  $(q_2, s_2) \in \mathcal{Q}^{A \times S}$  with the apply rule of the accessible product:

$$\frac{q_1 @ q \rightarrow q_2 \in \Delta^A \quad s_1 @ s \rightarrow s_2 \in \Delta^S \quad \frac{T'_1}{(q_1, s_1) \in \mathcal{Q}^{A \times S}} \quad \frac{T'}{(q, s) \in \mathcal{Q}^{A \times S}}}{(q_2, s_2) \in \mathcal{Q}^{A \times S}}$$

For the inverse direction of the apply rules, and using the induction hypothesis, we will be able to infer  $(q_2, s_2) \in \mathcal{Q}^{A \widehat{\times} S}$  with some  $T'_1$  and  $T'$  and ending with the following proof tree:

$$\frac{q_1 @ q \rightarrow q_2 \in \Delta^A \quad s_1 @ s \rightarrow s_2 \in \Delta^S \quad \frac{T'_1}{(q_1, s_1) \in \mathcal{Q}^{A \widehat{\times} S}} \quad \frac{T'}{(q, s) \in \mathcal{Q}^{A \widehat{\times} S}}}{(q_2, s_2) \in \mathcal{Q}^{A \widehat{\times} S}}$$

**Lemma 20.**  $q_1 @ q \rightarrow q_2 \in \Delta^{\widehat{scl}_S(A)}$  iff  $q_1 @ q \rightarrow q_2 \in \Delta^{scl_S(A)}$ .

*Proof.* Following the same logic in Lemma 15, this lemma holds by the following sequence of rules, for some proof trees  $T_1$ ,  $T$ ,  $T'_1$  and  $T'$  :

$$\frac{q_1 @ q \rightarrow q_2 \in \Delta^A \quad s_1 @ s \rightarrow s_2 \in \Delta^S \quad \frac{T_1}{(q_1, s_1) \in \mathcal{Q}^{A \widehat{\times} S}} \quad \frac{T}{(q, s) \in \mathcal{Q}^{A \widehat{\times} S}}}{q_1 @ q \rightarrow q_2 \in \Delta^{\widehat{scl}_S(A)}}$$

$$\frac{q_1 @ q \rightarrow q_2 \in \Delta^A \quad s_1 @ s \rightarrow s_2 \in \Delta^S \quad \frac{T'_1}{(q_1, s_1) \in \mathcal{Q}^{A \times S}} \quad \frac{T'}{(q, s) \in \mathcal{Q}^{A \times S}}}{(q_1, s_1) @ (q, s) \rightarrow (q_2, s_2) \in \Delta^{A \times S}}$$

$$\frac{(q_1, s_1) @ (q, s) \rightarrow (q_2, s_2) \in \Delta^{A \times S}}{q_1 @ q \rightarrow q_2 \in \Delta^{\widehat{scl}_S(A)}}$$

For the inverse direction, the sequence of rules, for some proof trees  $T_1$ ,  $T$ ,  $T'_1$  and  $T'$  will be:

$$\frac{q_1 @ q \rightarrow q_2 \in \Delta^A \quad s_1 @ s \rightarrow s_2 \in \Delta^S \quad \frac{T_1}{(q_1, s_1) \in \mathcal{Q}^{A \times S}} \quad \frac{T}{(q, s) \in \mathcal{Q}^{A \times S}}}{(q_1, s_1) @ (q, s) \rightarrow (q_2, s_2) \in \Delta^{A \times S}}$$

$$\frac{(q_1, s_1) @ (q, s) \rightarrow (q_2, s_2) \in \Delta^{A \times S}}{q_1 @ q \rightarrow q_2 \in \Delta^{\widehat{scl}_S(A)}}$$

$$\frac{q_1 @ q \rightarrow q_2 \in \Delta^A \quad s_1 @ s \rightarrow s_2 \in \Delta^S \quad \frac{T'_1}{(q_1, s_1) \in \mathcal{Q}^{A \widehat{\times} S}} \quad \frac{T'}{(q, s) \in \mathcal{Q}^{A \widehat{\times} S}}}{q_1 @ q \rightarrow q_2 \in \Delta^{\widehat{scl}_S(A)}}$$

**Proof of Correctness of Theorem 2.** For the proof of theorem for nested words with *SHA*, we extend the instantiation of the rule system for schema-based cleaning from Fig. 25 with  $\det(A)$ , yielding the rule system in Fig. 26.

$$\begin{array}{c}
 \frac{Q \in \diamond^{\Delta^{det(A)}} \quad s \in \diamond^{\Delta^S}}{Q \in \diamond^{\Delta^{\widehat{scl}_S(det(A))}} \quad (Q, s) \in \mathcal{Q}^{det(A)\widehat{\times}S}} \\
 \\
 \frac{Q_1 @ Q \rightarrow Q_2 \in \Delta^{det(A)} \quad s_1 @ s \rightarrow s_2 \in \Delta^S \quad (Q_1, s_1) \in \mathcal{Q}^{det(A)\widehat{\times}S} \quad (Q, s) \in \mathcal{Q}^{det(A)\widehat{\times}S}}{Q_1 @ Q \rightarrow Q_2 \in \Delta^{\widehat{scl}_S(det(A))} \quad (Q_2, s_2) \in \mathcal{Q}^{det(A)\widehat{\times}S}}
 \end{array}$$

Fig. 26: Extending the instantiation of the alt. definition of schema-based cleaning:  $\widehat{scl}_S(det(A)) = (\Sigma, \mathcal{Q}^{\widehat{scl}_S(det(A))}, \Delta^{\widehat{scl}_S(det(A))}, I^{\widehat{scl}_S(det(A))}, F^{\widehat{scl}_S(det(A))})$ .

The whole instantiation holds with the previous instantiation for words and we can still identify the rule system for  $\widehat{scl}_S(det(A))$  with the rule system  $det_S(A)$ . With the same identification of judgements and predicate renaming, the two systems are still exactly the same. Having  $\widehat{scl}_S(det(A)) = det_S(A)$  implies, by Proposition 17  $scl_S(det(A)) = det_S(A)$ .  $\square$