Inference of Shape Expression Schemas
from Typed RDF Graphs

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Abstract
We consider the problem of constructing a Shape Expression Schema (ShEx) that describes
the structure of a given input RDF graph. We employ the framework of grammatical inference,
where the objective is to find an inference algorithm that is both sound i.e., always producing
a schema that validates the input RDF graph, and complete i.e., able to produce any schema,
within a given class of schemas, provided that a sufficiently informative input graph is
presented. We study the case where the input graph is typed i.e., every node is given with its
types. We limit our attention to a practical fragment ShEx0 of Shape Expressions Schemas
that has an equivalent graphical representation in the form of shape graphs. We investigate
the problem of constructing a canonical representative of a given shape graph. Finally,
we present a sound and complete algorithm for shape graphs thus showing that ShEx0 is
learnable from typed graphs.

1 Introduction
Traditionally, in relational databases defining the schema is the mandatory first step before a
database can be even populated with data. Novel database models, such as NoSQL and graph
databases, quite intentionally allow to store and process data without declaring any schema in
order not to hinder the natural evolution of the database structure while the applications around it
are being developed. In fact, often a suitable schema formalism is proposed long after a particular
database model has established its place in practice. In those circumstances a natural problem
of schema inference arises: given a schema-less database construct a schema that captures the
structure of the database. This problem has been identified as an important research direction
and is well motivated since the knowledge of database structure is instrumental in any meaningful
data processing tasks such as querying or transformation.

In the present paper, we present a principled approach to the problem of inference of schema
for graph databases. We consider RDF graphs and Shape Expression Schemas (ShEx) [41, 37].
ShEx builds on the success of XML Schema and allows to describe the structure of an RDF graph
by defining patterns of arrangement of RDF nodes. More precisely, ShEx specifies a collection of
node types, each type defined by a regular expression that constrains the types of the outbound

1
neighborhood of a node. Take for instance the RDF graph storing bug reports, presented in Figure 1 together with its shape expression schema. The schema requires a bug report to have a

![RDF graph with bug reports](image)

Figure 1: An RDF graph with bug reports (top right) together with a shape expression schema (bottom) and the corresponding shape graph (top left). str is a built-in type for literal string nodes.

description and a user who submitted it. Optionally, a bug report may have an employee who verified it. Also, a bug report can have a number of related bug reports. A user has a name and an optional email address while an employee has a name and a mandatory email address. We point out that just like with XML Schema the nodes of the RDF graph need not by typed and it is the task of a validation algorithm to find for a valid node typing \([33, 26, 37]\), and furthermore, some nodes may need to have more than one type e.g., emp needs to have the types User and Employee.

We focus our investigation on a practical subclass ShEx that allows type definitions with collections of atoms with multiplicities ranging over 1, ?, +, and *, and does not allow disjunction or grouping. ShEx is particularly suited to capture the topology of RDF graphs obtained by exporting relational databases in a number of formalisms proposed for this task, such as R2RML, Direct Mapping, and YARRRML [36, 35, 3]. Also, ShEx has a significant overlap with an alternative schema language for RDF, the Shape Constraint Language (SHACL) [8]. More importantly, the class ShEx enjoys a useful and sought-after feature of having an equivalent graphical representation in the form of a shape graph, where nodes are types and edges are labeled by both a symbol and a multiplicity (cf. Figure 1).

In this paper, we present our findings on learning shape graphs from typed graphs, graphs whose nodes come with type informations. Indeed, in RDF there is the predicate rdf:type, which is the dedicated element of standard vocabulary intended for the purpose of assigning types to nodes of the graph. In out work we assume that the typing that assigns to every node a set of its types, is given in a manner independent of the graph. As an example the typed version of
the graph in Figure 1 is presented in Figure 2. Consequently, the problem of schema inference is reduced to inferring type definitions. This problem may seem trivial because in fact it is simple to solve when nodes have precisely one type. For instance, if we consider in Figure 2 all nodes that have type User, then the definition of this type is straightforward since all nodes have an outgoing name edge leading to a node whose type is precisely str and some nodes have an outgoing email edge that also leads to a node whose type is unambiguously str. Hence, the type definition User → name: str, email: str?

The inference of type definition is, however, less obvious when the nodes have multiple types: when inferring type definition we need to make choice of the relevant type. For instance consider the nodes of type Bug and notice that bug₁ has an outgoing edge verifiedBy that leads to a node emp₁ that has both types User and Employee. Depending on the choice the definition of Bug can become either

\[ \text{Bug} \rightarrow \text{descr: str, submittedBy: User, verifiedBy: User?, related: Bug*} \]

or

\[ \text{Bug} \rightarrow \text{descr: str, submittedBy: User, verifiedBy: Employee?, related: Bug*} \]

Naturally, these two definitions are not equivalent and the question is which one should be chosen. We find that the second type definition is more appropriate for two reasons. First, we observe that Employee ⊆ User i.e., every node that has the type Employee will also have the type User. Indeed, this can be established by observing the typed graph alone: there is no node that has type Employee and not User (while the converse is true: there are node that have type User but not Employee). Secondly, should the type User be used in the context of the edge verifiedBy, then we should be able to find an edge verifiedBy that leads to a node that has only the type User. In general, our algorithm for constructing the appropriate type definitions is based on a comprehensive analysis of the typing information present in the input typed graph.

More importantly, our approach is a solution to the inference problem stated with the use of grammatical inference framework [23], which in recent years has been successfully applied to a number of database formalisms ranging from queries [11, 38] to schemas [5, 10] to transformations [28, 27]. In essence, an inference algorithm needs to be both sound i.e., producing a schema
that validates the input graph, and complete i.e., able to infer any goal schema with a sufficiently informative input graph, typically referred to as characteristic graph of the goal language of typed graphs.

In this paper, we present an algorithm that is both sound and complete for the full class of shape graphs (ShEx). Interestingly, our investigations into learnability lead us to study the problem of canonization. Namely, for a given shape graph there might be a large number of equivalent shape graphs that define the same language of typed graphs. When presented with a characteristic graph, the inference algorithm outputs one of the shape graphs that define the goal language. It is desirable for the algorithm to output the same shape graph regardless of how the characteristic graph is constructed and returning the canonical representative is an elegant approach to address this need. Consequently, we present an effective characterization of canonical shape graphs based on a canonization procedure and design our inference algorithm in such a way that it too returns the canonical shape graph that defines the goal language.

This paper is organized as follows. In Section 2 we present basic notions. In Section 3 we define the framework of grammatical inference for shape graphs. In Section 4 we present basic instruments for analyzing the input typed graph. In Section 5 we investigate the problem of canonization of shape graphs. In Section 6 we present a sound and complete inference algorithm for shape graphs from typed graphs. In Section 7 we discuss the related work. Finally, in Section 8 we summarize our findings and outline future directions of study.

2 Basic notions

Throughout this paper we employ elements of function notation to relations. For instance, for a binary relation \( R \subseteq A \times B \) we set \( \text{dom}(R) = \{ a \in A \mid \exists b \in B. \ (a,b) \in R \} \), \( \text{ran}(R) = \{ b \in B \mid \exists a \in A. \ (a,b) \in R \} \), \( R(a) = \{ b \in B \mid (a,b) \in R \} \) for \( a \in A \), and \( R^{-1}(b) = \{ a \in A \mid (a,b) \in R \} \) for \( b \in B \).

Intervals. We use the standard notation \([n; m]\) to denote intervals, which represent nonempty sets of consecutive natural numbers with \(0 \leq n \leq m \leq \infty \). The value \( n \) (resp. \( m \)) is called the minimum of the interval (resp. the maximum). By \( I \) we denote the set of all intervals although our schema formalisms use only basic intervals \( M = \{0, ?, 1, *, +\} \) for which we employ a shorthand notation: \( 0 \) is \([0; 0]\), \( ? \) is \([0; 1]\), \( 1 \) is \([1; 1]\), \( * \) is \([1; \infty]\), and \( + \) is \([0; \infty]\).

We employ the point-wise addition operation \([n_1; m_1] + [n_2; m_2] = [n_1 + n_2; m_1 + m_2]\) and the natural interpretation of the inclusion relation \([n_1; m_1] \subseteq [n_2; m_2]\) if \( n_2 \leq n_1 \) and \( m_1 \leq m_2 \). Finally, we define the function \( \text{fit} \) that maps any set \( X \) of natural numbers (occurrences) into a smallest interval in \( I \) that contains all elements of \( X \).

Graphs. We assume a fixed and finite set \( \Sigma \) of edge labels and a fixed and finite set of types \( \Gamma \).

Definition 2.1 (Graph) A graph \( G \) is a pair \((N_\mathcal{G}, E_\mathcal{G})\), where \( N_\mathcal{G} \) is a set of nodes and \( E_\mathcal{G} \subseteq N_\mathcal{G} \times \Sigma \times N_\mathcal{G} \) is a set of oriented labeled edges.

For an edge \( e = (n, a, m) \) we set \( \text{source}(e) = n, \text{lab}(e) = a, \) and \( \text{target}(e) = m \). Also, for a node \( n \) of a graph \( G \) we identify its set of outbound edges \( \text{out}_G(n) = \{ e \in E_\mathcal{G} \mid \text{source}(e) = n \} \).

Definition 2.2 (Shape graph) A shape graph \( S \) is a function \( \text{arity}_S : \Gamma \times \Sigma \times \Gamma \rightarrow M \) that validates the input graph, and complete i.e., able to infer any goal schema with a sufficiently informative input graph, typically referred to as characteristic graph of the goal language of typed graphs. By ShEx we denote the set of all shape graphs.

The semantics of shape graphs is defined with the notion of typings that associate to nodes of a graph set of types.
any node with type typing

The set of all finite typed graphs \( G \) is a graph extended with a proper typing (w.r.t. a shape graph). The language \( L \) iff there is a witness \( \lambda \) satisfies \( t \) of a graph

We employ the framework of grammatical inference \([23]\) to inference of ShEx schemas from typed graphs. In essence, this framework require the existence of a learning algorithm capable of inferring every schema from a sufficiently informative input typed graph. Such a typed graph is called characteristic and to avoid collusion the inference algorithm is required be conservative: it must infer the goal schema even if to the characteristic graph we add other potentially less
informative fragments. Formally, $G$ extends $G'$ consistently with schema $S$ iff there is $G''$ such that $G = G' \sqcup G''$ and $G, G', G'' \in L(S)$.

**Definition 3.1** Shape graphs are learnable from typed graphs in polynomial time iff there is a polynomial inference algorithm learner such that

**Soundness** For every input typed graph $G \in G_4$ the inference algorithm returns a shape graph learner($G$) = $S$ such that $G \in L(S)$.

**Completeness** For every shape graph $S \in \text{ShEx}_0$ there exists a characteristic graph $G \in L(S)$ such that for any $G' \in L(S)$ we have learner($G \sqcup G'$) = $S$. □

### 4 Typed graphs

In this section we introduce tools for inspecting typed graphs and extracting the relevant typing information for inference algorithm. Throughout this section we fix a shape graph $S$.

**Contexts and type definition fragments.** As we illustrate next, when inferring a type definition, we only need to inspect the local outbound neighborhood of nodes of the type in question, we can ignore the identity of nodes and focus on types alone. More importantly, the definition of type can be inferred in fragments independently for each outgoing edge label.

**Example 4.1** Take the graph $G_0$ in Figure 4.1 and the typing corresponding to the presented embedding of $G_0$ in $S_0$. Consider the type $U$ with its 3 nodes in $G_0$: $u_1$, $u_2$, and $e_1$, and fix the outgoing edge label to $n$. In this context, which we denote $C_0 = (U, n)$, each of the nodes has precisely one outgoing edge that leads to literal node of type $\text{str}$. Naturally, when constructing a schema $S$ this should yield the corresponding type definition fragment $S(C_0) = \text{str}^1$. Analogously, for the context $C_1 = (U, e)$ the corresponding fragment should be $S(C_1) = \text{str}^1$ since not every node has an outgoing $e$-edge.

Now, consider the type $B$ and some of its contexts. For the context $C_2 = (B, r)$, we get quite naturally $S(C_2) = B^*$. For $C_3 = (B, a)$ we observe that in the graph $G_0$ whenever a node has type $E$, it also has type $U$, which indicates the type inclusion $E \subseteq U$. Consequently, the type fragment for $C_3$ should be $S(C_3) = U^1$ rather than $U^1E^*$ for which there is insufficient evidence (such as a node of type $B$ with two outgoing $a$-edges). Finally, for $C_4 = (B, v)$ two type definition fragments can be considered $U^1$ and $E^*$. Given the (scarce) evidence the reasonable choice seems $S(C_4) = E^*$ since the former option $U^1$ would be justified if there was a node of type $B$ with an outgoing $v$-edge leading to a node having the type $U$ only. □

Formally, a context is a pair $(t, a) \in \Gamma \times \Sigma$. If $\Gamma = \{t_1, \ldots, t_k\}$, a type definition fragment is a string of the form $t_1^{\mu_1} \ldots t_k^{\mu_k}$, where $\mu_i \in M$ for $1 \leq i \leq k$. In the sequel, we abuse the notation
and for a context \( C = (t, a) \) write \( \text{arity}^C_S(s) = \text{arity}_S(t, a, s) \) if \( (t, a, s) \in E_S \) and \( \text{arity}^C_S(s) = 0 \) otherwise. Then the type definition fragment corresponding to a context \( C \) in shape graph \( S \) is
\[
S(C) = t_1^{\text{arity}^C_S(t_1)} \cdots t_k^{\text{arity}^C_S(t_k)}.
\]

In the sequel, we denote by \( \text{minarity}_S \) and \( \text{maxarity}_S \) respectively the minimum and the maximum value of \( \text{arity}_S \) respectively.

**Inspecting graphs and graph languages.** The previous example also shows that the information relevant to inferring a given type definition fragment boils down to counting occurrences in the input graph. Because the nodes of a typed graph are assigned sets of types, we first identify all possible sets of types

\[
\text{Typesets}(S) = \{\text{typing}_G(n) \mid G \in L(S), n \in N_G\}.
\]

We point out that \( \text{Typesets}(s) \) can be constructed effectively by identifying all sets of types that have nonempty intersection, which is known to be decidable [39].

Now, for a context \( C = (t, a) \), a graph \( G \), and a typeset \( T \in \text{Typesets}(S) \) we define the interval that contains the number of nodes having precisely types \( T \) in the context \( C \)
\[
\text{occur}^C_G(T) = \text{fit}_M(\{\{m \in N_G \mid (n, a, m) \in E_G, \text{typing}_G(m) = T\} \mid n \in N_G, t \in \text{typing}_G(n)\}).
\]

We extend the above construction to nonempty sets of typesets \( \mathcal{T} \subseteq \text{Typesets}(G) \)
\[
\text{occur}^C_G(\mathcal{T}) = \text{fit}_M(\{\{m \in N_G \mid (n, a, m) \in E_G, \text{typing}_G(m) \in \mathcal{T}\} \mid n \in N_G, t \in \text{typing}_G(n)\}).
\]

Finally, for a type \( t' \) we count its occurrences as
\[
\text{occur}^C_G(t') = \text{fit}_M(\{\{m \in N_G \mid (n, a, m) \in E_G, t' \in \text{typing}_G(m)\} \mid n \in N_G, t \in \text{typing}_G(n)\}).
\]

In the sequel, we denote by \( \text{minoccur}^C_G(x) \) and \( \text{maxoccur}^C_G(x) \) the minimal and the maximal value of \( \text{occur}^C_G(x) \). Also, we extend the above notation to a language defined by a shape graph \( S \) as \( \text{occur}^S_G(x) = \text{occur}_{\text{str}(S)}^S(x) \). Naturally, our goal is to find useful connections between \( \text{occur} \) that can be observed in examples and \( \text{arity} \) that is in the shape graph. These connections can, however, be quite involved.

**Example 4.2 (cont’d. Example 4.1)** Take the schema \( S_0 \) in Figure 4.1. For the contexts that lead to a node with a single type, such as \( C_0 = (U, n) \), \( C_1 = (U, e) \), and \( C_2 = (B, r) \), the correspondence between \( \text{occur} \) and \( \text{arity} \) is straightforward e.g.,
\[
\text{occur}^S_{C_0}(\text{str}) = \text{arity}^S_{C_0}(\text{str}) = 1 \quad \text{occur}^S_{C_1}(\text{str}) = \text{arity}^S_{C_1}(\text{str}) = * \quad \text{occur}^S_{C_0}(B) = \text{arity}^S_{C_0}(B) = *
\]

For \( C_3 = (B, s) \) and \( C_4 = (B, v) \) which lead to nodes with possibly both types \( U \) and \( E \), their mutual relationship \( E \subseteq U \) renders the connections between \( \text{arity}_S \) and \( \text{occur}_S \) far from obvious.

\[
\begin{align*}
\text{arity}^S_{C_3}(U) &= 1 & \text{occur}^S_{C_3}(\{U\}) &= ? & \text{arity}^S_{C_3}(U) &= 0 & \text{occur}^S_{C_3}(\{U\}) &= 0 \\
\text{arity}^S_{C_3}(E) &= 0 & \text{occur}^S_{C_3}(\{U, E\}) &= ? & \text{arity}^S_{C_3}(E) &= ? & \text{occur}^S_{C_3}(\{U, E\}) &= ? & \square \\
\text{occur}^S_{C_3}(\{E\}) &= 0 & \text{occur}^S_{C_3}(\{E\}) &= 0
\end{align*}
\]

**Connections between type occurrences and its arity in shape graph.** We now state a number of results that allow to establish connections between occurrences of types in the input typed graph and the arities in the goal schemas. Naturally, these connections are the basis of the work of our inference algorithm.

First, we observe that type containment can be easily derived from a typed graph.
Proposition 4.3 For any two types \( t_1 \) and \( t_2 \) we have that \( t_1 \subseteq t_2 \) if and only if for every \( T \in \text{Typesets}(S) \) we have \( t_1 \in T \Rightarrow t_2 \in T \).

The appropriate connections between occurrences of a type and its arity in the schema can be established in the presence of a sufficiently informative graph, which we define next.

Definition 4.4 (Weakly characteristic graph) A typed graph \( G \) is weakly characteristic of schema \( S \) if the following conditions are satisfied:

- for every \( T \in \text{Typesets}(S) \), there is a node in \( G \) whose types are precisely \( T \);
- for every context \( C \in \Gamma \times \Sigma \) and every typeset \( T \in \text{Typesets}(S) \), there is a node that has exactly \( \text{arity}_S(C)(T) \) edges that goes to a node with types \( T \), and another node that has exactly \( \text{maxarity}_S(C)(T) \); if \( \text{maxarity}_S(C)(T) = \infty \), we require at least \( |T| + 1 \) such edges.

We point out that its size may be exponential in the size of the goal schema and the results on the sizes of counter-examples of containment of shape graphs \([39]\) show that this bound is tight.

We also point out that a weakly characteristic graph may contain insufficient amount of information to infer the goal schema but it will allows us to establish important links between \( \text{occur} \) and arity. First we state the link for the minimum values.

Proposition 4.5 For a weakly characteristic graph \( G \) for \( S \), a context \( C \), and a type \( t \) we have \( \text{minoccur}_G^C(t) = \sum \{ \text{arity}_S(C)(t') \mid t' \subseteq t \} \).

A less obvious link for maximum values is stated next.

Proposition 4.6 For a weakly characteristic graph \( G \) for \( S \) and a typeset \( T \in \text{Typesets}(S) \), \( \text{maxoccur}_G^C(t) \geq |T| + 1 \) if there is \( t \in T \) with \( \text{maxarity}_S(C)(t) = \infty \), and \( \text{maxoccur}_G^C(t) = \sum \{ \text{maxarity}_S(C)(t') \mid t' \subseteq T \} \) otherwise.

Finally, we point out important connection for equivalent types.

Proposition 4.7 For any type \( t \) take the set of equivalent types \( T = \{ t' \mid t = t' \} \). Then for any shape graph \( S' \) that is equivalent to \( S \), we have that \( \sum_{s \in T} \text{arity}_S(s) = \sum_{s \in T} \text{arity}_{S'}(s) \).

5 Canonization of shape graphs

The connections between \( \text{arity} \) and \( \text{occur} \) are however more intricate than even the above example suggests due to the fact that there might be many equivalent shape graphs.

Example 5.1 In this example we consider 3 pairs of equivalent shape graphs presented in Figure 7 and focus on a single context \( C = (s, a) \). For the schemas \( S_1 \) and \( S'_1 \) we observe that \( t_1 = t_2 \), which gives the equivalence of the type definition fragments \( S_1(C) = t_1^1 t_2^1 = t_1^2 t_2^2 = S'_1(C) \). For the schemas \( S_2 \) and \( S'_2 \) we observe that \( t \subseteq t_1 \cup t_2 \cup t_3 \), which renders equivalent the fragments \( S_2(C) = t^1 t_1^1 t_2^1 t_3^1 = t^1 t_1^2 t_2^2 = S'_2(C) \). Finally, we observe that \( S_3(C) = t^1 t_1^1 t_2^1 t_3^1 = t^1 t_1^2 t_2^2 = S'_3(C) \) because \( t \setminus (t_1 \cup t_2) = t' \setminus (t_1 \cup t_2) \).

When a complete inference algorithm is presented with a characteristic graph of a goal schema for which a number of equivalent formulations exists, a well-behaved algorithm returns a formulation chosen according to clear rules. These rules define a method of constructing a canonical shape graph that we present next. Because this method needs to choose a single type among groups of equivalent types, we facilitate this choice by fixing a total ordering \( < \) of the set of types \( \Gamma \). Also, by \( \text{arity} \) and \( \text{maxarity} \) we denote the lower and upper bound of the interval of \( \text{arity} \), and we introduce similar shortcuts for \( \text{occur} \).
We next show that the exhaustive application of the rule (R1) ensures equality of the minimums of each arity.

**Claim 5.4.1** $S_1 \equiv S' \equiv S_2$.  

We next show that the exhaustive application of the rule (R1) ensures equality of the minimums of each arity.

**Claim 5.4.2** For any context $C$ and any type $t$ we have $\text{minarity}^C_{S_1}(t) = \text{minarity}^C_{S_2}(t)$.

The exhaustive application of the rule (R2) ensures that each infinite maximum arity is the same.

**Claim 5.4.3** For any context $C$ and any type $t$ we have $\text{maxarity}^C_{S_1}(t) = \infty$ iff $\text{maxarity}^C_{S_2}(t) = \infty$.

Finally, the exhaustive application of the rule (R3) guarantees that the multiplicities 0, $\omega$, and 1 are the same.

**Claim 5.4.4** For any context $C$ and any type $t$ if $\text{maxarity}^C_{S_1}(t) < \infty$ or $\text{maxarity}^C_{S_2}(t) = \infty$, then $\text{maxarity}^C_{S_1}(t) = \text{maxarity}^C_{S_2}(t) = \infty$. 

Figure 7: Equivalent shape graphs: $S_1 \equiv S'_1$, $S_2 \equiv S'_2$, and $S_3 \equiv S'_3$. 

**Definition 5.2** Take a shape graph $S \in \text{ShEx}_o$. We define the canonization operations of $S$ w.r.t. a context $C \in \Gamma \times \Sigma$.

(R1) if $t = t'$, $t < t'$, $\text{minarity}(t) = 0$, and $\text{minarity}(t') = 1$, then set $\text{minarity}(t) = 1$ and $\text{minarity}(t') = 0$;

(R2) if $t \subseteq t_1 \cup \ldots \cup t_k$ and $\text{maxarity}(t_i) = \infty$ for every $1 \leq i \leq k$, then set $\text{maxarity}(t) = \infty$;

(R3) if $t \setminus (t_1 \cup \ldots \cup t_k) \equiv t' \setminus (t_1 \cup \ldots \cup t_k)$, $t < t'$, $\text{arity}(t') = 0$, $\text{arity}(t) = \omega$, and $\text{maxarity}(t_i) = \infty$ for every $1 \leq i \leq k$, then set $\text{arity}(t) = 0$ and $\text{arity}(t') = \omega$.

By $\text{Can}^<(S)$ we denote the shape graph obtained by applying exhaustively the rule (R1) in every context, then exhaustively the rule (R2) in every context, and finally, exhaustively the rule (R3) in every context. We say that $S$ is canonical w.r.t. $\text{Can}^<(S) = S$.

**Example 5.3 (cont’d. Example 5.1)** $S'_1$ is obtained from $S_1$ by applying the rule (R1) since $t_1$ and $t_2$ are equivalent. $S'_2$ is obtained from $S_2$ by applying the rule (R2) because $t$ is covered by $t_1$, $t_2$, and $t_3$ i.e., $t \subseteq t_1 \cup t_2 \cup t_3$. Finally, $S'_3$ is obtained from $S_3$ by applying the rule (R3) because $t \setminus (t_1 \cup t_2) = t' \setminus (t_1 \cup t_2)$. 

We next state and prove the main result of this section.

**Theorem 5.4** For any two $S \equiv S'$ we have $\text{Can}^<(S) = \text{Can}^<(S')$.

Below, we outline the proof of the above theorem and we assume a fixed order $<$ on types, fix two schemas $S$ and $S'$, assume that they are equivalent $S \equiv S'$, and let $S_1 = \text{Can}^<(S)$ and $S_2 = \text{Can}^<(S')$. It is relatively straightforward to show that each of the canonization operations preserves the semantics.

**Claim 5.4.1** $S_1 \equiv S \equiv S' \equiv S_2$.  

We next show that the exhaustive application of the rule (R1) ensures equality of the minimums of each arity.

**Claim 5.4.2** For any context $C$ and any type $t$ we have $\text{minarity}^C_{S_1}(t) = \text{minarity}^C_{S_2}(t)$.

The exhaustive application of the rule (R2) ensures that each infinite maximum arity is the same.

**Claim 5.4.3** For any context $C$ and any type $t$ we have $\text{maxarity}^C_{S_1}(t) = \infty$ iff $\text{maxarity}^C_{S_2}(t) = \infty$.

Finally, the exhaustive application of the rule (R3) guarantees that the multiplicities 0, $\omega$, and 1 are the same.

**Claim 5.4.4** For any context $C$ and any type $t$ if $\text{maxarity}^C_{S_1}(t) < \infty$ or $\text{maxarity}^C_{S_2}(t) = \infty$, then $\text{maxarity}^C_{S_1}(t) = \text{maxarity}^C_{S_2}(t) = \infty$. 

9
6 Inference of Shape Graphs

We now present the inference algorithm for typed graphs. Because of space restrictions, we only present its outline on the graph in Figure 5 and the contexts in Example 4.1. The detailed algorithm can be found in appendix.

For a given graph $G$ the algorithm typed-learner performs the following steps.

1. It begins by gathering the typesets present in the input graph $\mathcal{T} = \{\text{types}_G(n) \mid n \in N_G\}$. In our example
   $$\mathcal{T} = \{\{\mathcal{B}\}, \{\mathcal{U}\}, \{\mathcal{U}, \mathcal{E}\}, \{\text{str}\}\}$$

2. It uses the existing evidence to establish the inclusion relationship between the types $t \subseteq s$ is assumed to hold iff for every $T \in \mathcal{T}$ we have that $t \in T$ implies $s \in T$. In our example
   $$\text{str} \subseteq \text{str}, \mathcal{E} \subseteq \mathcal{E}, \mathcal{E} \subseteq \mathcal{U}, \mathcal{U} \subseteq \mathcal{U}, \mathcal{B} \subseteq \mathcal{B}.$$  

3. It fixes an order $\prec$ of enumerating the types $\Gamma$ that is compatible with $\prec$ and $\subseteq$: $t \prec s$ whenever $t \subseteq s$ or if $t$ and $s$ are incomparable by $\subseteq$ and $t < s$. In our example we set
   $$\text{str} \prec \mathcal{E} \prec \mathcal{U} \prec \mathcal{B}.$$  

4. For every context $C$ it enumerates the types used in this context in the order $\prec$ and infers the minimal arities: $\text{minarity}(t) = \text{minoccur}(t) - \sum_{s \subseteq t} \text{minarity}(s)$. In our example
   $$\text{minarity}^C_G(\mathcal{B}) = 0, \quad \text{minarity}^C_G(\mathcal{E}) = 0, \quad \text{minarity}^C_G(\mathcal{U}) = 1, \quad \text{minarity}^C_G(\mathcal{E}) = 0, \quad \text{minarity}^C_G(\mathcal{U}) = 0.$$  

5. For every context $C$ it enumerates the types used in this context in the reversed order $\prec^{-1}$ and infers the maximal arity according to one of the following cases:

   (a) If $\text{maxoccur}(T) \geq |T| + 1$ for all typesets $T \in \mathcal{T}$ containing $t$, then it sets $\text{maxarity}(t) = \infty$; In our example, this applies to $\text{maxarity}^C_G(\mathcal{B}) = \infty$.

   (b) Otherwise, if $\text{minarity}(t) = 1$, then it sets $\text{maxarity}(t) = 1$; In our example, this applies to $\text{maxarity}^C_G(\mathcal{U}) = 1$.

   (c) Otherwise, it looks for a typeset $T$ that characterizes $t$ for $C$, in the sense that $T$ contains only $t$ and types $s$ with $t \subseteq s$, and sets $\text{maxarity}(t) = \text{maxoccur}(T) - \sum_{s \in T \setminus \{t\}} \text{maxarity}(s)$. In our example,
   $$\text{maxarity}^C_G(\mathcal{E}) = 0 \quad \text{because } \{\mathcal{U}, \mathcal{E}\} \text{ characterizes } \mathcal{E} \text{ for } C_3,$$
   $$\text{maxarity}^C_G(\mathcal{U}) = 0 \quad \text{because } \{\mathcal{U}\} \text{ characterizes } \mathcal{U} \text{ for } C_4,$$
   $$\text{maxarity}^C_G(\mathcal{E}) = 1 \quad \text{because } \{\mathcal{U}, \mathcal{E}\} \text{ characterizes } \mathcal{E} \text{ for } C_4.$$

   (d) If there does not exist a typeset $T$ that characterizes $t$ (typically when $t$ is a union of other types), $t$ is said to be obfuscated for $C$. In which case, we look for typesets $T_i$ that contains $t$ and that have $\text{maxarity}^C_S(t) \neq \inf$ for all $t \in T_i$. If there is only one such $T_i$, then we set $\text{maxarity}^C_G(t) = 1$ if
   $$\text{maxoccur}^C_G(T) - \sum \{\text{maxarity}^C_G(t') \mid t' \in T, t' > t\} - \sum \{\text{minarity}^C_G(t') > 0 \mid t' \in T, t' < t\},$$
and we set $\maxarity^C_G(t) = 0$ otherwise.

If there are more than one such $T_i$, we pick any two typesets $T_1$ and $T_2$. We compute $N = \sum_{t' \in T_1 \setminus \{t\}} \maxarity^C_G(t')$. We set $\maxarity^C_G(t) = 0$ if $\maxoccurrence^C_G((T_1, T_2)) - N = \sum_t (\maxoccurrence^C_G(T_i) - N)$, otherwise, we set $\maxarity^C_G(t) = 1$.

6. Finally, the result may not be consistent with the input graph, in particular if the graph is not characteristic. The algorithm therefore has to check consistency for all type definitions, and relax locally all type definitions which are not consistent.

The notion of characteristic graph $G$ for shape graph $S$ is central. As explained before, we require the graph $G$ to be weakly characteristic for $S$. This will allow to give enough information to infer the canonical representative of $S$ unless $S$ has obfuscated types.

If there are obfuscated types, we need to add extra information to the characteristic graph. For every context $C$, and type $t$ that is obfuscated for $C$, we consider all typesets $T_i$ that contain $t$ and such that $\maxarity^C_G(t) \neq \infty$. We denote the set of such typesets by $\cover(t)$. Now, a graph $G$ is characteristic for $S$ if it is weakly characteristic for $S$ and if for every type $t$ obfuscated for a context $C = (t_0, a)$ with $|\cover(t)| \geq 2$, for every pair $\{T_1, T_2\} \subseteq \cover(t)$, there is a node $n$ of type $t_0$ such that the number of $a$-labelled edges that go to a node that has $T_1$ or $T_2$ as a typing is maximal, i.e. is equal to $\sum_{t' \in T_1 \cup T_2} \maxarity^C_G(t')$.

**Theorem 6.1** ShEx$_0$ is learnable in polynomial time from typed graphs.

We claim that if the input graph is characteristic for a shape graph $S$, the algorithm outputs $Can(S)$. We outline the proof of the completeness below.

1. The algorithm gathers the correct typeset as each typeset that may exist is present in the graph.

2. The algorithm computes the correct inclusion relation between types, because $s \subseteq t$ implies that $(t \in T \Rightarrow s \in T)$ for any typeset $T$, and if $s \nsubseteq t$, then there exists a typeset $T$ that contains $t$ but not $s$, and this typeset is present in a characteristic graph.

3. Minimal arities are computed correctly. This is proved recursively: for minimal types (i.e. types that contains no other types), we directly have $\minoccurrence^C_G(t) = \minarity^C_G(t)$. For larger types, $\minoccurrence^C_G(t) = \minarity^C_G(t) + \sum_{s \subseteq t} \minarity^C_G(s)$, and hence $\minarity^C_G(t) = \minoccurrence^C_G(t) - \sum_{s \subseteq t} \minarity^C_G(s)$.

4. For maximal arities, there are four cases.

   (a) If $\maxarity^C_G(t) = \infty$, then evidence of it can be found in a characteristic graph. Indeed, for a typeset $T$, if $\maxoccurrence^C_G(T) \geq |T| + 1$, that means that there is a type $t \in T$ for which $\maxarity^C_G(t) = \infty$. For a type $t$, if we consider a typeset $T$ that contains only smaller types $s \subset t$, then either $t$ of some $s \in T \setminus \{t\}$ has an infinite maximal arity. But in a canonical shape graph $S$, if this happens for all $T$ that contain $t$, then also $\maxarity^C_G(t) = \infty$.

   (b) Other case is when $\maxarity^C_G(t) \neq \infty$. Then, if $\minarity^C_G(t) = 1$, then it implies that $\maxarity^C_G(t) = 1$.

   (c) It remains only cases where $\arity^C_G(t) \in \{0, ?\}$. If there is a typeset $T$ that contains only $t$ and its super-types, we can do as for minimal arities and use the fact that $\maxoccurrence^C_G(t) = \maxarity^C_G(t) + \sum \{\maxarity^C_G(s) \mid s \supseteq t\}$ (note that all $s$ have finite arity).
strong equivalence

The first relation, there exists a host of research on schemas for semistructured (graph) data [10, 18] and their versions of finite automata (probabilistic, Glushkov, etc.) and then rewrite them into regular expressions. In [21, 14, 13]) the author also propose a many applications of this technique are based on (bi)simulation [17, 42, 25, 40], often taking into account particular queries that are to be answered. In [21] the author also propose a quotient-based method but introduce two equivalence relations that are not based on bisimulation. The first relation, strong equivalence, requires similarity of the structure of incoming and outgoing

7 Related work

There exists a host of research on schemas for semistructured (graph) data [10, 18] and their inference [24, 32, 31]. Dataguides [24] are data structures that represent all paths in semistructured graph but it is assumed that graph have entry points, essentially root nodes, which is not an assumption we make for RDF graphs. [31] the typing is by a datalog program, the typings allow objects to have multiple types at the same time which is essential when the data is fairly irregular. Approximate merging of types using clustering algorithms is applied until the typing is of acceptable size.

Several approaches have been proposed for inference of schemas for tree-structured data [20, 30, 15]. XTract [20] infers DTD schemas by generating candidate regular expressions for each element name and then selecting the best one. Another method is to generate various versions of finite automata (probabilistic, Glushkov, etc.) and then rewrite them into regular expressions [6, 15]. Inference of more expressive schema formalisms such as unranked tree automata or XML Schema is considered in [4, 12, 33, 19]. These approaches also include inference of schema for JSON data [3, 4] that by inferring types of each node by merging the types of their children in a manner analogous to deterministic.

Another relevant areas of research is graph summarization, where the goal is to compute compact but accurate representation of the input graph. One approach is to compute quotient graph w.r.t. an equivalence relation by collapsing nodes in the same equivalence class into one. Many applications of this technique are based on (bi)simulation [17, 42, 25, 40], often taking into account particular queries that are to be answered. In [21] the author also propose a quotient-based method but introduce two equivalence relations that are not based on bisimulation. The first relation, strong equivalence, requires similarity of the structure of incoming and outgoing

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edges, and *weak equivalence*, which requires similarity between incoming or outgoing edges. We point out that often the approaches make the assumption of one type per node, which simplifies the type definition process. \cite{22} follows this line of research presenting four other summaries that are representable in the style of E-R diagrams together with efficient algorithms for their computation. In \cite{29} graph summaries are computed based on estimating the frequency with which subgraphs match given query patterns. The paper \cite{2} presents an approach where users first define a *structuredness* function $\sigma$ that measures how well a given RDF graph fits to the schema and then discover a partitioning of the entities of an RDF graph into subsets which have high structuredness. They consider an optimization variant of the inference problem: finding the lowest number of types for a given threshold on $\sigma$ or finding a fixed number of types that maximizes $\sigma$. This approach as most others can be described as *pragmatic*, the goal is to find a schema that is as small as possible and describes the data with a good precision. Our motivations, in contrast, are more fundamental and aim at understanding the inherent limitations of inference.

8 Conclusions and future work

In the present paper we have studied the problem of inference of shape expression schemas for typed RDF graphs. We have presented a sound and complete inference algorithm for a practical subclass ShEx$_0$ of shape expressions schemas. Our investigation lead us to study the canonization problem for ShEx$_0$ and we present an effective canonization procedure for ShEx$_0$.

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