Inference of Shape Graphs for Graph Databases

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Abstract

We investigate the problem of constructing a shape graph that describes the structure of a given graph database. 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 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 identify a number of fundamental limitations that preclude feasible inference. We present inference algorithms based on natural approaches that allow to infer schemas that we argue to be of practical importance.

2012 ACM Subject Classification Information systems → Graph-based database models

Keywords and phrases RDF, Schema, Inference, Learning, Fitting, Minimality, Containment.

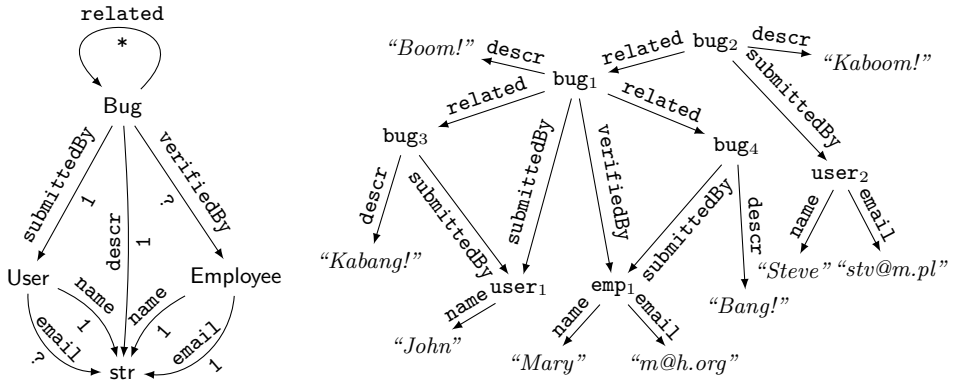
Digital Object Identifier 10.4230/LIPIcs.ICDT.2022.7

Funding *Piotr Wieczorek*: This author has been partially supported by Polish National Science Center grant NCN 2016/23/B/ST6/01438.

1 Introduction

Traditionally, in relational databases, defining the schema is the mandatory first step before a database can even be populated with data. However, novel database models, such as graph databases, quite intentionally allow to store and process data without declaring any schema. This facilitates the evolution of the structure of a database while the applications around it are being developed. In fact, often a suitable schema formalism is proposed 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 [1] and is well motivated since the knowledge of database structure is instrumental in any meaningful data processing task such as querying or transformation.

In the present paper, we present a principled approach to the problem of schema inference for graph databases. We consider RDF graphs and Shape Expression Schemas (ShEx) [55, 47]. 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 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 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



Bug → `descr` : str, `submittedBy` : User, `verifiedBy` : Employee?, `related` : Bug*
User → `name` : str, `email` : str?
Employee → `name` : str, `email` : str

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.

nodes of the RDF graph need not be typed and it is the task of a validation algorithm to find a valid node typing [42, 35, 47]. Furthermore, some nodes may need to be assigned more than one type, for instance the node $\texttt{emp}_1$ needs to satisfy the types User and Employee.

We focus our investigation on a practical subclass ShEx_0 that defines types with collections of atoms with *arities* ranging over `1`, `?`, `+`, and `*`. This fragment does not allow disjunction or union types but can adequately approximate schemas with those features. ShEx_0 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 [46, 45, 13]. More importantly, the class ShEx_0 enjoys a sought-after feature of an equivalent graphical representation in the form of a *shape graph* whose nodes are types and edges are labeled by a symbol and a multiplicity (see Figure 1).

We present a principled approach to the problem of graph database schema inference, where we start with the fundamental question: *What is an inference algorithm?*. We answer it using the framework of *grammatical inference* [28], which in recent years has been successfully applied to a number of database formalisms ranging from queries [17, 48] to schemas [7, 22] and transformations [38, 36]. In essence, an inference algorithm needs to be both *sound*, i.e., produce a schema that validates the input graph, and *complete*, i.e., able to infer any goal schema with a sufficiently informative input graph. This formal framework allows us to tackle another fundamental question: *When is inference feasible?* Indeed, we identify classes of schemas that are not learnable, which reveals two principal challenges in schema inference: 1) distinguishing unbounded arities `*` and `+` from bounded ones `1` and `?`, and 2) distinguishing recursive types from their finite non-recursive unravelings.

A suitable ShEx_0 inference algorithm needs to identify the types and their definitions. ShEx_0 assigns to every node of a graph a set of types by using the notion of *embedding*, which is an extension of the standard graph simulation. Consequently, our first attempt is to use graph simulation to identify sets of nodes whose *outbound* neighborhood shares structural similarity, and therefore, should have the same type. Interestingly, this approach yields a very reasonable inference algorithm that generalizes the structural information of the input graph, and in particular, easily introduces recursion in the constructed schema. The generalization is however very eager, and in particular, the algorithm clumps together any two types that are related by subtype relation such as Employee $\subseteq$ User where every node of

type Employee has also type User. Indeed, this inference algorithm produces a shape that is *singular*, having no two types that cannot be distinguished with the help of simulation, and consequently it prohibits schemas with subtypes like the schema in Figure 1.

To address this shortcoming we investigate using the *context* in which nodes are used: their *inbound* neighborhood. Indeed, the nodes of type User and the nodes of type Employee are used in different contexts, although their use may partially overlap e.g., the node $\texttt{emp}_1$ is used both as an employee and as a user. An inference algorithm based on using context information constructs a schema that belongs to the class of *deterministic* shape graph, which permits every edge label to be present at most once in a type definition. This class of schemas is incomparable with singular shape graph. For instance, the schema in Figure 1 is deterministic but is not singular. We find, however, that an indiscriminate use of the context information leads to *overfitting*, and in particular, it may fail to introduce recursion and may produce voluminous schemas. It appears that an inference algorithm must choose carefully the information to identify the set of types. We propose, as a proof of concept, a hybrid inference algorithm that extends the simulation-based approach with a modest amount of context information that consists of a single incoming edge. This algorithm produces schemas that are *context-singular*, a generalization of singular schemas that allows subtyping between types used in different contexts.

Finally, we survey a number of graph databases and inspect their schemas. Our analysis shows that ShEx_0 and the proposed subclasses lack certain features present in real-world schemas, most notably union types, but we can approximate them very well. This makes our algorithms an excellent solution for preparing the first draft of a schema to be refined by a knowledgeable architect.

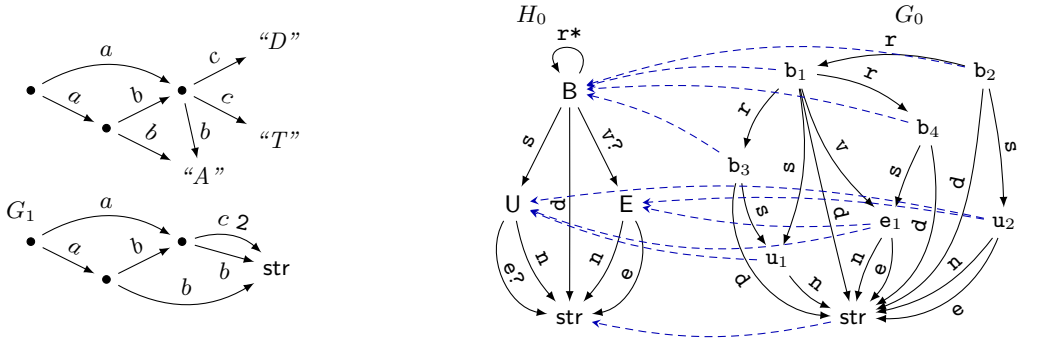
Organization. The paper is organized as follows. In Section 2 we present basic notions, including shape graphs and their embeddings. In Section 3 we formally state the problem of inference. In Section 4 we present a simulation-based inference algorithm for the class of singular shape graphs. In Section 5 we present negative implications of unrestrained use of context information in inference. In Section 6 we propose a hybrid approach combining the simulation-based approach with elements of context information. In Section 7 we present an analysis of schemas of a number of graph databases. We discuss related work in Section 8. We summarize our findings and outline future research directions in Section 9.

2 Basic notions

Throughout this paper we apply a functional notation to relations, and conversely, often view functions as relations. For instance, for a binary relation $R \subseteq A \times B$ we set $\mathsf{dom}(R) = \{a \in A \mid \exists b \in B.\ (a,b) \in R\}$, $\mathsf{ran}(R) = \{b \in B \mid \exists a \in A.\ (a,b) \in R\}$, $R(a) = \{b \in B \mid (a,b) \in R\}$ 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 $[i;j]$ for $0 \leq i \leq j \leq \infty$ to denote *intervals* that represent nonempty sets of consecutive natural numbers. By I_0 we denote the set of all intervals. Our schema formalisms use only four *basic intervals* (M_0) given with their shorthand notation: 1 is $[1;1]$, ? is $[0;1]$, + is $[1;\infty]$ and * is $[0;\infty]$. A *simple interval* has the form $[i;i]$ for $0 \leq i < \infty$, and often we use i for $[i;i]$. Throughout this paper, we employ the point-wise addition operation $[i_1;j_1] \oplus [i_2;j_2] = [i_1+i_2;j_1+i_2]$. A set of intervals M is *proper* if any interval is contained in an interval in M. For a proper M we define the function fit_M that maps any finite nonempty set of natural numbers (occurrences) into a smallest interval in M containing it.

Graphs and schemas. We employ a generic model of a graph that we use to model both RDF and the subclass ShEx_0 that allows type definitions consisting of collections of atoms using basic intervals [47, 49]. Our methods do not inspect data values of literal nodes, and consequently, we will abstract them using their type alone but this requires us to record the number of some types of edges as illustrated in Figure 2a.



(a) An RDF graph (above) and its abstraction as a simple graph (below)

(b) An embedding $G_0 \preccurlyeq H_0$ (concise versions of graphs from Figure 1).

Figure 2 Graphs and embeddings.

When drawing graphs we typically omit the label 1 and simple intervals are denoted with natural numbers e.g., 2 stands for $[2;2]$ which indicates two identical edges. We point out a dichotomy of node kinds and their types: literal nodes can only have literal types and non-literal nodes can only have non-literal types. While it might be tempting to remove literal types from consideration and focus on data-free graphs, we keep literal types and nodes because without them it is difficult to define reasonable schema families without subtypes.

We assume a finite set Σ of edge labels and an enumerable set of node identifiers $\mathcal{N} = \mathcal{U} \cup \mathcal{L}$, where $\mathcal{U}$ is an infinite set of identifiers used to represent both URIs and blank nodes, and $\mathcal{L}$ is a finite set of types of literal nodes e.g., str representing strings. We assume that $\mathcal{U} \cap \mathcal{L} = \emptyset$.

▶ **Definition 1.** *A* graph *G is a triple $(N_G, E_G, \mathsf{arity}_G)$, where $N_G \subseteq \mathcal{N}$ is a finite set of nodes, $E_G \subseteq (N_G \cap \mathcal{U}) \times \Sigma \times N_G$ is a set of labeled oriented edges, and arity_G maps every edge to an interval. A* shape graph *is a graph that uses only basic intervals and by ShEx_0 we denote the set of all shape graphs. A* simple graph *is a graph that assigns to every edge a simple interval and this simple interval is 1 unless the edge leads to a node in $\mathcal{L}$. By G_0 we denote the set of simple graphs. A simple graph G is* data-free *if $N_G \cap \mathcal{L} = \emptyset$.* □

In Figure 2b we present a more concise version of the graphs from Figure 1 adapted to our graph model. For $M \subseteq \mathsf{M}_0$, we write $\mathsf{ShEx}_0(M)$ to restrict the choice of arities to M. For an edge $e = (n, p, m)$ we let $\mathsf{source}(e) = n$, $\mathsf{lab}(e) = p$, and $\mathsf{target}(e) = m$. For a given node n of G we identify its outbound neighborhood $\mathsf{out}_G(n) = \{e \in E_G \mid \mathsf{source}(e) = n\}$. Given two graphs G_1 and G_2 by $G_1 \uplus G_2$ we denote their disjoint union. In the sequel, we often refer to shape graphs as *schemas* and their nodes as *types*. We also abuse the standard tree terminology and say that nodes n and n' are siblings if there is a node m that has outgoing edges to n and to n'.

Embeddings. We recall next, and illustrate in Figure 2b, the notion of embedding that allows to define the semantics of shape graphs as schemas [49] and is instrumental in our inference methods. Here, by id_A we denote the identity relation on a given set A.

▶ **Definition 2** (Embedding). *[49] An* embedding *of a graph G in a graph H is a binary*

relation $R \subseteq (N_G \times N_H) \cap (\mathcal{U} \times \mathcal{U} \cup \mathsf{id}_{\mathcal{L}})$ *such that for any* $(n, m) \in R$ *there exists a* witness *of embedding of* n *in* m *w.r.t.* R*, i.e., a function* $\lambda : \mathsf{out}_G(n) \to \mathsf{out}_H(m)$ *such that*

1. *for every* $e \in \mathsf{out}_G(n)$ *we have that* $\mathsf{lab}(e) = \mathsf{lab}(\lambda(e))$*,*
2. *for every* $f \in \mathsf{out}_H(m)$ *we have that* $\bigoplus\{\mathsf{arity}_G(e) \mid \lambda(e) = f\} \subseteq \mathsf{arity}_H(f)$*, where* $\bigoplus$ *stands for the point-wise sum of all the intervals.*
3. *for every* $e \in \mathsf{out}_G(n)$ *we have that* $(\mathsf{target}(e), \mathsf{target}(\lambda(e))) \in R$*.*

The embedding R *is* total *if* $\mathsf{dom}(R) = N_G$*. We write* $G \preccurlyeq H$ *if there exists a total embedding of* G *in* H*. An* autoembedding *of* G *is an embedding of* G *in itself.* □

Figure 2b presents an example of the embedding between the concise versions of RDF graph and the shape graph in Figure 1. It is known that there exists exactly one *maximal embedding* between two graphs [47] (since the union of embeddings is also an embedding), and constructing maximal embeddings between pairs of shape graphs and between simple graphs and shape graphs is in P [49]. In the sequel, by $\ll_{G:H}$ we denote the maximal embedding of G in H, by $\ll_G$ the maximal autoembedding of G, and we use both relation symbols using infix notation. The *language* of a shape graph H is $L(H) = \{G \in \mathsf{G_0} \mid G \preccurlyeq H\}$. We recall from [49], that embeddings can be composed, and in particular, $G \preccurlyeq H$ implies $L(G) \subseteq L(H)$, but the converse does not necessarily hold as illustrated in Figure 3.

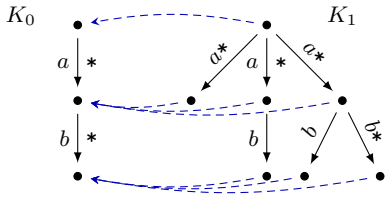


Figure 3 Containment does not imply an embedding: K_0 and K_1 are equivalent but $K_1 \preccurlyeq K_0$ and $K_0 \not\preccurlyeq K_1$.

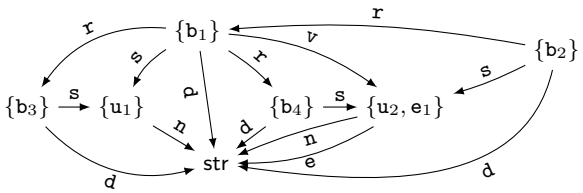


Figure 4 Aggregate of G_0 by grouping P_0 induced by the bisimulation relation of G_0.

Throughout the paper we use the following terminology. A simple graph G *satisfies* a shape graph H, and H *recognizes* G, iff $G \in L(H)$. Two shape graphs H and K are *equivalent*, in symbols $H \equiv K$, iff $L(H) = L(K)$. A node n of a simple graph G *has type* t of a shape graph H iff $n \ll_{G:H} t$. Given two types t_1 and t_2 of a shape graph H, a type t_1 is a *subtype* of t_2, in symbols $t_1 \subseteq_H t_2$, iff $\forall G \in L(H).\ \forall n \in N_G.\ n \ll_{G:H} t_1 \Rightarrow n \ll_{G:H} t_2$. Finally, a type t of H is *recursive* iff it is part of a loop in H.

3 Inference of shape graphs

In this section we introduce the framework of grammatical inference, present a number of limit point arguments that help to identify main challenges in inferring shape graphs, and finally, we present the construction of graph aggregation that we use to infer shape graphs.

3.1 Grammatical inference

In this paper we investigate the problem of *shape graph inference*, which consists of constructing a shape graph for a given input simple graph. To this end we adopt the framework of *grammatical inference* [28], which has originally been proposed for word languages and has been successfully applied to a number of database formalisms ranging from queries [17, 48] to schemas [7, 22] to transformations [38, 36]. In essence, the framework

requires the inference algorithm to be capable of inferring any goal schema given a sufficiently informative input. We are interested in inference from positive data: the input consists of a graph that belongs to the goal language. To prevent collusion, namely a solution where a characteristic input graph encodes the goal schema using an elaborate scheme, the inference algorithm is required to be robust under extension: it must infer the goal schema even if the characteristic graph is accompanied by other potentially less informative graphs that satisfy the schema. Formally, G *extends* G' *consistently with schema* H iff there is G'' such that $G = G' \uplus G''$ and $G, G', G'' \in L(H)$.

▶ **Definition 3.** *A class of shape graphs* $\mathcal{C}$ *is* learnable *from a class of graphs* $\mathcal{G}$ *iff there is an inference algorithm* $\mathsf{learner}$ *such that*

Soundness *For every input graph* $G \in \mathcal{G}$ *the inference algorithm returns a schema* $\mathsf{learner}(G) = H$ *such that* $H \in \mathcal{C}$ *and* $G \in L(H)$.

Completeness *For every goal schema* $H \in \mathcal{C}$ *there exists a* characteristic graph $G_H \in L(H)$ *such that for any* G *that extends* G_H *consistently with* H *we have* $\mathsf{learner}(G) \equiv H$.

Furthermore, we say that $\mathcal{C}$ *is* learnable in polynomial time *if the inference algorithm works in polynomial time. We also say that* $\mathcal{C}$ *is* learnable in polynomial data *if there exists a polynomial that bounds the size of the characteristic graph as a function of the size of the goal schema.* □

As an illustrative example of grammatical inference consider the problem of inferring basic intervals M_0 from a given sample of its members $\{i_1, \ldots, i_k\}$. Take the function $\mathsf{fit}_{\mathsf{M}_0}$ that returns the smallest basic interval that contains all the elements given on the input. Naturally, $\mathsf{fit}_{\mathsf{M}_0}$ is a sound inference algorithm since it returns an interval that contains all the elements given on the input. It is also a complete inference algorithm because we can construct characteristic samples for every element of M_0. For instance, for the goal interval $+ = [1; \infty]$ a characteristic sample is $\{1, 2\}$. Indeed, $\mathsf{fit}_{\mathsf{M}_0}(\{1, 2\}) = +$ but more importantly $\mathsf{fit}_{\mathsf{M}_0}(X) = +$ for any X subset of $[1; \infty]$ that includes $\{1, 2\}$.

Now, consider the full class of intervals I_0 and take the function $\mathsf{fit}_{\mathsf{I}_0}$ as a inference algorithm. It is naturally sound since $\mathsf{fit}_{\mathsf{I}_0}(X) = [\min(X); \max(X)]$ but it is not complete since it cannot infer an unbounded interval $[i_0; \infty]$ from a finite input set. In fact, I_0 is not learnable because one can show that there is no sound and complete inference algorithm for I_0 (from positive samples alone). Next, we present a general characterization of classes of languages that are not learnable. We will use it as a tool for identifying key challenges in schema inference.

3.2 Limit point

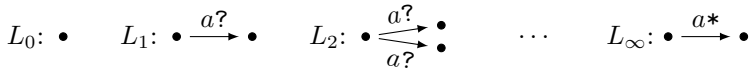
We recall that a class of languages $\mathcal{C}$ has the *limit point* property iff $\mathcal{C}$ contains an ascending chain of languages $L_1 \subsetneq L_2 \subsetneq \ldots$ whose limit point $L_\infty = \bigcup_i L_i$ also belongs to $\mathcal{C}$. It is a folklore result that the limit point property precludes learnability (from positive examples) [2]: essentially, no finite amount of examples from the goal language allows to distinguish between the limit point L_∞ and some language L_i in the ascending chain. We formally show that it also holds for the framework we adopt in this paper.

▶ **Proposition 4.** *No class of shape graphs with the limit point property is learnable from simple graphs.*

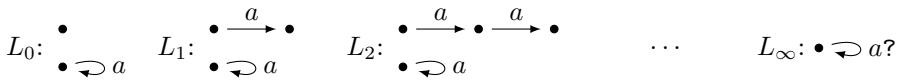
The limit point argument allows us to identify a number of limitations of inference of shape expressions schemas.

▶ **Lemma 5.** *For any $M \subseteq \{1, ?, *, +\}$ with at least two elements the class $\mathsf{ShEx}_0(M)$ has the limit point property.*

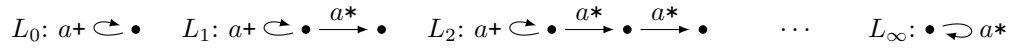
Proof sketch. It suffices to consider sets of 2 multiplicities and in Figure 5 we present three cases. The limit point arguments for all remaining cases are constructed very similarly to



(a) Limit point for $\mathsf{ShEx}(?, *)$



(b) Limit point for $\mathsf{ShEx}(1, ?)$.



(c) Limit point for $\mathsf{ShEx}(*, +)$.

Figure 5 Limit points for various subclasses of ShEx_0

$\mathsf{ShEx}(?, *)$ in Figure 5a (details in appendix). □

Consequently, we obtain the following corollary.

▶ **Corollary 6.** ShEx_0 *is not learnable from simple graphs.*

A closer look at the limit point arguments offers an insight into the reasons why inferring ShEx_0 is not feasible. Firstly, we observe in Figure 5a that one of the challenges in distinguishing between L_i and L_∞ is in deciding based on finite input example when to use unbound arity $*$ as opposed to $?$ (similar argument holds for $+$ and $?$, etc.). Secondly, in Figures 5b and 5c we observe an analogous difficulty in deciding between other pairs of arities, but more importantly, we also observe a different difficulty: whether to choose a simple recursive type (L_∞) or allow some arbitrary non-recursive unfolding of it (L_i). To summarize, the constructions in Figure 5 point to two key challenges of inferring shape schemas for graph databases: 1) distinguishing between bounded and unbounded arities, and 2) introducing recursive types especially from a possibly acyclic input example.

3.3 Graph aggregate

The inference algorithms that we propose in this paper construct schemas with an operation that generalizes the standard graph quotient. Recall that the graph quotient operation essentially reduces to a single node every set of nodes that are equivalent w.r.t. a given equivalence relation. In the context of schema inference, we are interested in grouping together nodes that we deem to have the same type but we point out that the underlying relation "*n and m are deemed to have the same type*" needs not be transitive in general. In fact, we do not even assume that this relation is reflexive because we may wish to intentionally ignore nodes of the input graph that we do not find informative enough.

▶ **Definition 7.** *A* node grouping *of a simple graph $G = (N_G, E_G, \mathsf{arity}_G)$ is a collection $P \subseteq 2^{N_G}$ of sets of nodes of G such that any $N \in P$ with $N \cap \mathcal{L} \neq \emptyset$ is a singleton. Given a proper set of intervals M, the* aggregate *of G by P w.r.t. M, in symbols $G \div_M P$, is the*

shape graph $H = (N_H, E_H, \mathsf{arity}_H)$*, where*

$$N_H = P,$$
$$E_H = \{(N, a, N') \in P \times \Sigma \times P \mid \exists (n, a, n') \in E_G,\ n \in N \wedge n' \in N'\},$$
$$\mathsf{arity}_H(N, a, N') = \mathsf{fit}_M\left(\left\{\bigoplus\{\mathsf{arity}_G(n, a, n') \mid n' \in N',\ (n, a, n') \in E_G\} \mid n \in N\right\}\right).$$

The requirement $N \cap \mathcal{L} \neq \emptyset$ follows from the dichotomy of node kinds and their types. To ensure that the aggregate is technically a (shape) graph, we assume that any subset of $\mathcal{N}$ is also a node identifier and for any $\ell \in \mathcal{L}$ we interpret $\{\ell\}$ as ℓ. In the sequel, when the set of intervals M is known from the context, we omit it in the aggregate and simply write $G \div P$.

In essence, for a given input graph G, our inference algorithms explore the lattice $(\mathcal{P}_G, \sqsubseteq)$ of all node groupings $\mathcal{P}_G$ of G from $P_\bot = \{\{n\} \mid n \in N_G\}$ to $P_\top = \{N_G \setminus \mathcal{L}\} \cup \{\{\ell\} \mid \ell \in N_G \cap \mathcal{L}\}$. The structure of this lattice is consistent with the containment relation: $P_1 \sqsubseteq P_2$ iff $G \div P_1 \subseteq G \div P_2$. This connection to containment is essential for guiding inference algorithms with characteristic graphs. When the goal schema is $G \div P$ for a node grouping P then for every relevant $P' \sqsubseteq P$ the characteristic graph needs to contain an example showing $G \div P' \not\supseteq G \div P$.

▶ **Example 8.** Consider G_0 and H_0 in Figure 2b, and take the node grouping that corresponds to the typing of G_0 w.r.t. H_0: $P = \{\{\mathtt{b}_1, \mathtt{b}_2, \mathtt{b}_3, \mathtt{b}_4\}, \{\mathtt{u}_1, \mathtt{u}_2, \mathtt{e}_1\}, \{\mathtt{e}_1\}, \{\mathsf{str}\}\}$. The aggregate $G_0 \div_{\mathsf{M}_0} P$ is in fact (equivalent to) H_0. □

The above example shows that G_0 carries sufficient information that with the right partition allows to infer the goal schema H_0.

The task is to identify a method that allows to group nodes of the input graph that are deemed to have the same type and at the same time can introduce unbounded arities and recursion in type definitions. A natural attempt at grouping nodes of a graph would be to use bisimulation. But as we illustrate in Figure 4 this fails to introduce unbounded arities and recursive types. In fact, it has been studied in the literature [27] and found to fail to generalize appropriately the input graph.

4 Singular shape graphs

In this section we address the two key challenges of inference by grouping nodes with the help of graph simulation relation. This yields an inference algorithm for a subclass of singular shape graphs. The inference algorithm allows to infer unbounded arities and recursive types even from acyclic input graph. The price is the ability to distinguish types from their subtypes.

Shape graphs assign types to nodes using an embedding, which is an adaptation of the standard notion of graph simulation. Consequently, we explore an approach of grouping together nodes that are comparable with the simulation relation. To that effect, for a given simple graph G we construct the graph $G*$ by changing the arity of every edge to $*$, and then, any autoembedding of $G*$ is a simulation relation on G and vice versa. Hence, we use the maximal autoembedding $\ll_{G*}$ to assess the relative amount of schema information that a node supplies: if $m \ll_{G*} n$, we consider m to provide no more schema information than n does. We introduce useful short-hands. We say that n *sim-dominates* m iff $m \ll_{G*} n$ and $m \neq n$. Also, n *properly sim-dominates* m is n *sim-dominates* m and $n \not\ll_{G*} m$. We say that n and m are *sim-equivalent* if $m \ll_{G*} n$ and $n \ll_{G*} m$. Finally, a node is *sim-maximal* if it is sim-dominated only by sim-equivalent nodes.

Using simulation to group nodes has an important drawback: the inability to distinguish types from their subtypes. Indeed, if $t_1 \subseteq t_2$, then any node that has type t_1 is simulated by nodes of type t_2 that characterize the type t_2. We return to this problem in Section 6 where we show how to handle inference of restricted cases of subtypes. We point out that permitting arbitrary subtypes allows to construct ascending chains, which can be then easily used in limit point arguments, as evidenced for instance in Figure 5b. This allows us to conclude that inferring subtypes is inherently problematic. Furthermore, we show that even forbidding subtypes does not suffice to guarantee learnability.

▶ **Proposition 9.** *Let* $\mathsf{FlatShEx}_0$ *be the subclass of shape graphs where no two different types are comparable by the containment relation. For any subset* $M \subseteq \mathsf{M}_0$ *with at least two elements* $\mathsf{FlatShEx}_0(M)$ *is not learnable.*

Consequently, stronger restrictions are needed and we propose the class of singular schemas whose types can all be distinguished with the graph simulation relation.

▶ **Definition 10.** *A type* t *of a shape graph* H *is* singular *iff* t *is not sim-dominated by any type in* H*. A shape graph is* singular *iff it has only singular types and by* $\mathsf{SinShEx}_0$ *we denote the set of all singular shape graphs.*

Intuitively, singularity ensures that for any two types t_1 and t_2, there exist nodes of type t_1 that can be distinguished from all nodes of type t_2 with the help of simulation. In the following example we show that simulation needs to be used carefully when identifying groups of nodes of the same type.

▶ **Example 11.** To keep the example simple, we limit the intervals used in shape graphs to $\{1, ?, *\}$. In figures we use a dotted green arrow $n \dashleftarrow m$ to indicate that n sim-dominates m. Take the graph G_2 in Figure 6, identify its sim-maximal nodes $Max = \{n_0, n_1, n_2, \mathsf{str}\}$, and consider the node grouping $P_0 = \{\{n_0\}, \{n_1\}, \{n_2\}, \{\mathsf{str}\}\}$. This grouping is too sparse: the aggregate $G_2 \div P_0$ does not recognize G_2. Consider then the grouping where every sim-maximal node is accompanied by all sim-dominated nodes: $P_{\max} = \{\{n_0\}, \{n_1, n_3\}, \{n_2, n_4\}, \{\mathsf{str}\}\}$. While $G_2 \div P_{\max}$ recognizes G_2, it is not singular because $\{n_0\} \ll_{G_2 \div P_{\max}*} \{n_2, n_4\}$. Although originally n_0 was sim-maximal, afterwards it became subsumed by the group $\{n_2, n_4\}$. It is then absorbed by $\{n_2, n_4\}$ and we get the node grouping $P^+_{\max} = \{\{n_1, n_3\}, \{n_0, n_2, n_4\}, \{\mathsf{str}\}\}$, which yields the singular shape graph H_2 that recognizes G_2.

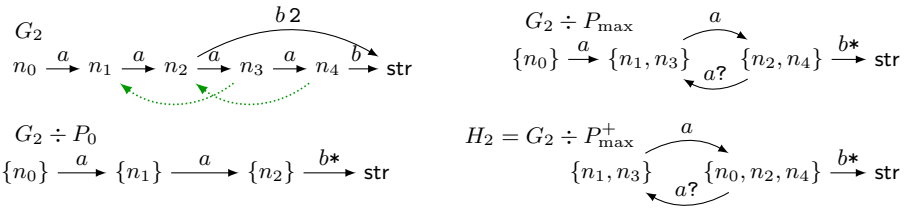


Figure 6 Example of inference using graph simulation. $G_2 \div P_0$ does not recognize G_2.

The node grouping $P_{\max}$ is not a good starting point for an inference algorithm because it might be overly eager as we illustrate next. Consider the graph G_3 in Figure 7. The node m_2 is sim-dominated by m_1 and m_3. The grouping $P_{\max} = \{\{m_0\}, \{m_1, m_2\}, \{m_2, m_3, m_4\}, \{\mathsf{str}\}\}$ forces $*$ on the edge from $\{m_0\}$ to $\{m_1, m_2\}$. It is, however, not necessary to add m_2 to any group: $P_1 = \{\{m_0\}, \{m_1\}, \{m_3, m_4\}, \{\mathsf{str}\}\}$ already yields H_3 that is singular, recognizes G_3, and is a tighter fit than $G_3 \div P_{\max}$. □

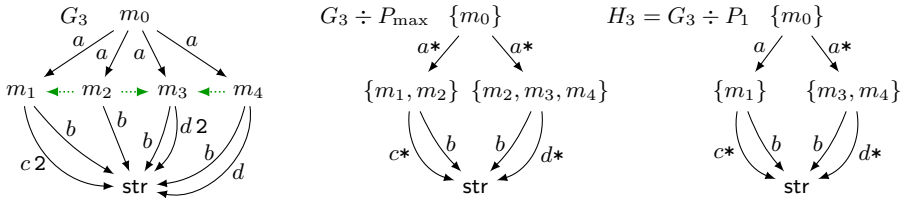


Figure 7 Example of inference using graph simulation. $G_3 \div P_{\max}$ is overgeneralized.

For inferring singular shape graphs we propose the algorithm sim-learner. It is parameterized by a proper set of intervals M which restricts the intervals used in the output singular shape graph. The algorithm constructs a node grouping P of the input graph G and it constructs

Algorithm 1 Inference algorithm for $\mathsf{SinShEx}_0(M)$

algorithm $\text{sim-learner}_M(G)$
input: $G = (N_G, E_G)$ a simple graph
param: M a proper set of intervals
output: inferred shape graph in $\mathsf{SinShEx}_0(M)$

begin
1: $Max := \{n \in N_G \mid \forall m \in N_G.\ n \ll_{G*} m \Rightarrow m \ll_{G*} n\}$
2: $P := \varnothing$
3: **for** $n \in Max$ **do**
4: $\quad P[n] := \{m \in Max \mid m \ll_{G*} n\}$
5: **while** $G \not\preccurlyeq G \div_M P$ **do**
6: $\quad$ Choose $n \in Max$ and $m \in N_G \setminus P[n]$ based on priority rules Φ, such that $m \ll_{G*} n$
7: $\quad$ add m to $P[n]$
8: **while** $\exists S, T \in P.\ S \neq T \wedge S \ll_{(G \div_M P)*} T$
9: $\quad$ merge S and T in P
10: **return** $G \div_M P$
end

only groupings where every sim-maximal node n belongs to precisely one node group, which can be accessed with a lookup operation $P[n]$. The algorithm begins by identifying all sim-maximal nodes (line 1) and grouping together all sim-equivalent nodes (lines 2-4). Next, as long as the aggregate $G \div_M P$ does not recognize the input graph, the algorithm iteratively identifies a node m that is absorbed by a node group $P[n]$ such that $m \notin P[n]$ (lines 5-7). Among all eligible pairs of m and $P[n]$ we choose one according to the following order Φ:

1. **siblings first** any m that has a sibling $n \in Max$ such that $P[n]$ contains all siblings of m that sim-dominate it.
2. **single choice** any m and $n \in Max$ such that all nodes that sim-dominate m are in $P[n]$.
3. **all else** any $n \in Max$ and $m \in N_G$ such that $m \in N_G \setminus P[n]$ and n sim-dominates m.

Finally, the algorithm merges any node groups that prevent the shape graph $G \div_M P$ from being singular (lines 8-10). We point out that the preference order Φ may indicate multiple equally preferred pairs and the algorithm may choose an arbitrary one: regardless of the choice the output always recognizes the input graph and when the input contains a characteristic graph, the algorithm will always converge on the goal schema. Φ prevents the algorithm sim-learner from performing unnecessary generalization: when executed on the graph G_3 in Figure 7 it returns the schema H_3. Furthermore, when run on G_2 in Figure 6 the algorithm returns the schema H_2, which illustrates that it is capable of inferring recursive

types even from acyclic input graphs.

In general the algorithm is sound for $\mathsf{SinShEx}_0$, but here we only claim that $\mathsf{sim\text{-}learner}_{1,*}$ is sound and complete for the shape graphs using 1 and $*$.

▶ **Theorem 12.** $\mathsf{SinShEx}_0(1,*)$ *is learnable in polynomial time and data from simple graphs.*

In Section 6.2 we take advantage of Φ to show completeness for a larger class but it remains an open question if the full class of singular shape graphs is learnable in polynomial time and data (but the existing evidence suggests it is unlikely [49]). The full class is however learnable with an algorithm that exhaustively explores the exponential space of possible singular shape graphs and uses an exponentially-large characteristic graph to help navigate this space.

▶ **Theorem 13.** $\mathsf{SinShEx}_0$ *is learnable from simple graphs.*

5 Deterministic shape graphs

In this section we investigate the potential ramifications of attempting to improve the process of identifying the set of types by exploiting the context in which nodes are used in the graph. More precisely, two nodes n and n' are used in the same *context* of node m and label a if there are two edges (m,a,n) and (m,a,n'), and in that case the nodes n and n' should have the same type. Such premise leads us to the class of deterministic shape expressions schemas that allow at most one type to be used in a given context.

▶ **Definition 14.** *A type t of a shape graph H is* deterministic *iff for every label $a \in \Sigma$ the type t has at most one outgoing edge with label a. A* deterministic *shape graph has only deterministic types and by* $\mathsf{DetShEx}_0$ *we denote the set of all deterministic shape graphs.*

Interestingly, the powerset method for determinization of finite automata can be adopted for inference of $\mathsf{DetShEx}_0$. We illustrate this algorithm in Figure 8 but refrain from formally introducing it because we do not wish to promote it in this paper. Later in this section we

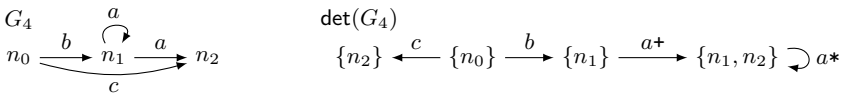


Figure 8 Determinization of a graph.

provide its alternative semantic characterization that will allow us to identify the pitfalls of an indiscriminate use of context information for shape graph inference.

Some caveats follow. Firstly, not every simple graph can be recognized by a deterministic shape graph. For instance, the graph G_1 in Figure 2a satisfies no deterministic schema because G_1 has a node with two outgoing b-edges, one of which leads to a literal node and the other to a non-literal node. Consequently, we limit the inputs to *data-free graphs*, simple graphs with no literal nodes. Secondly, the limit point in Figure 5b shows that $\mathsf{DetShEx}_0$ is not learnable, and thus, we recall from [49] a subclass $\mathsf{DetShEx}_0^-$ that we show learnable with the determinization algorithm. Formally, a *reference* to a type $t \in N_H$ is any edge $e \in E_H$ that leads to t i.e. $\mathsf{target}_H(e) = t$. A reference e is $*$*-closed* if $\mathsf{arity}_H(e) = *$ or all references to $\mathsf{source}_H(e)$ are $*$-closed. $\mathsf{DetShEx}_0^-$ is the class of deterministic shape graphs that do not use + and any type using ? is referenced at least once and all references to it are $*$-closed.

▶ **Theorem 15.** $\mathsf{DetShEx}_0$ *is not learnable from data-free graphs.* $\mathsf{DetShEx}_0^-$ *is learnable from data-free graphs in polynomial data.*

It can be proved (see appendix) that the determinization algorithm outputs the containment-minimal shape graph in $\mathsf{DetShEx}_0^-$ that satisfies the input data-free graph G. This makes the determinization algorithm an embodiment of the *minicon* principle which postulates for constructing the minimal consistent schema. This principle has a negative ramifications.

▶ **Proposition 16.** *For any n there exists a graph G_n of size quadratic in n such that the containment-minimal shape graph in $\mathsf{DetShEx}_0^-$ that validates G is of size exponential in n.*

We conclude that an indiscriminate use of the context information has negative impact on inference of shape graphs: the obtained schemas risk being too verbose and overfitted. Also, nontrivial classes of shape graphs are too rich to benefit from blindly following the minicon principle.

6 Hybrid approach

In this section we pursue a hybrid approach that extends the simulation-based approach with a limited amount of context information to enable inference of shape graphs with subtypes. We then identify the subclass that our hybrid algorithm is able to infer among shape graphs using arbitrary basic intervals.

6.1 Context-singular shape graphs

We extend the simulation-based approach with context information limited to the labels of incoming edges. This allows to infer subtypes as long as they are used in different contexts. For instance, this extension can infer the schema in Figure 1, where Employee $\subseteq$ User but Employee is used in the context of verifiedBy and User is used only in the context submittedBy.

Here, the contexts in which a type t is used in a shape graph H are described by the labels of incoming edges: $\mathit{ctx\text{-}lab}_H(t) = \{a \in \Sigma \mid \exists s \in N_H.\ (s, a, t) \in E_H\}$. Singularity of shape graph requires that no type is sim-dominated by another type. We relax this by allowing a sim-dominated type as long as it is used in at least one context where none of its sim-dominating types are.

▶ **Definition 17.** *Given a shape graph H, a type t of H is* context-singular *if and only if $\mathit{ctx\text{-}lab}_H(t) \not\subseteq \bigcup\{\mathit{ctx\text{-}lab}_H(t') \mid t' \in N_H,\ t \ll_{H*} t',\ t \neq t'\}$. H is* context-singular *if it has only context-singular types. $\mathsf{CtxSinShEx}_0$ is the set of all context-singular shape graphs.*

To adapt sim-learner to inference of context-singular shape graphs we introduce an uncoupling operation that for a given graph creates a distinct clone of a node for every of its incoming edges, so that all incoming edges of a node have the same label. Formally, the *uncoupling* of a graph G is $\bar{G} = (N_{\bar{G}}, E_{\bar{G}}, \mathsf{arity}_{\bar{G}})$, where

$$N_{\bar{G}} = \bigcup\{\mathit{uncouple}(n) \mid n \in N_G\},$$

$$\mathit{uncouple}(n) = \begin{cases} \{n\} & \text{if } n \in \mathcal{L}, \\ \{(\bot, n)\} & \text{if } \mathit{ctx\text{-}lab}_G(n) = \emptyset, \\ \{(a, n) \mid a \in \mathit{ctx\text{-}lab}_G(n)\} & \text{otherwise,} \end{cases}$$

$$E_{\bar{G}} = \{(\eta, a, \mathit{trg}(a, m)) \mid (n, a, m) \in E_G,\ \eta \in \mathit{uncouple}(n)\}$$

$$\mathit{trg}(a, m) = \begin{cases} m & \text{if } m \in \mathcal{L}, \\ (a, m) & \text{otherwise,} \end{cases}$$

$$\mathsf{arity}_{\bar{G}}(\eta, a, \mathit{trg}(a, m)) = \mathsf{arity}_G(n, a, m) \quad \text{for } (n, a, m) \in E_G \text{ and } \eta \in \mathit{uncouple}(n).$$

When each node has incoming edges with the same label, using the context information is simpler. For instance, a type t of an uncoupled shape graph H is context-singular iff there is no type t' such that $t \ll_{H*} t'$ and $ctx\text{-}lab_H(t) \subseteq ctx\text{-}lab_H(t')$. Consequently, for uncoupled graphs we define a contextualized variant of the autoembedding relation: $n \ll_K^{ctx} m$ iff $n \ll_K m$ and $ctx\text{-}lab_K(n) \subseteq ctx\text{-}lab_K(m)$. We adapt terminology and say that n *ctx-dominates* m iff $m \ll_K^{ctx} n$ and $n \neq m$. Also, n is *ctx-maximal* if any node that ctx-dominates n is also ctx-dominated by n.

Now, the inference algorithm hybrid-learner is a modification of sim-learner where we replace every occurrence of G by $\bar{G}$ and every occurrence of $\ll$ by $\ll^{ctx}$. We illustrate hybrid-learner on an example.

▶ **Example 18.** We run hybrid-learner in Figure 9 on the graph G_0 introduced in Figure 2. In the uncoupling of G_0 we indicate with $m \dashrightarrow n$ that $m \ll^{ctx}_{\overline{G_0}*} n$. In this example we use

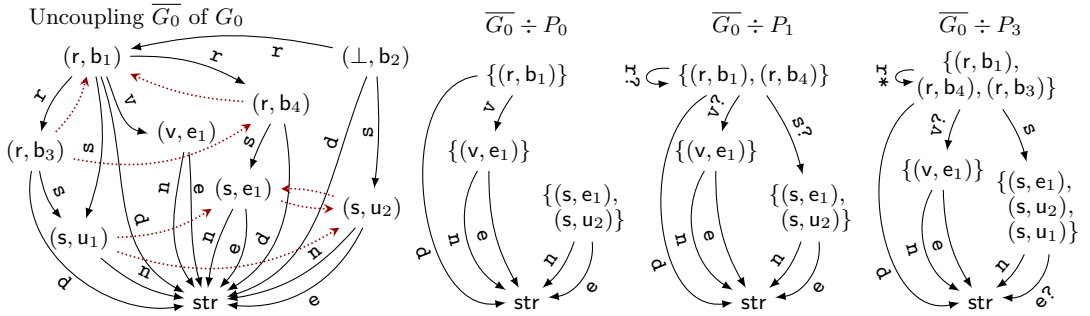


Figure 9 Execution of hybrid-learner on G_0. $m \dashrightarrow n$ means that n sim-dominates m.

the complete set of basic intervals $\mathsf{M}_0 = \{1, ?, +, *\}$. The algorithm begins with the node grouping $P_0 = \{\{(r, b_1)\}, \{(v, e_1)\}, \{(s, e_1), (s, u_2)\}, \{str\}\}$ obtained from the ctx-maximal nodes in $\overline{G_0}$. Because $\overline{G_0} \div P_0$ does not recognize $\overline{G_0}$, the algorithm uses Φ to identify nodes that can be absorbed: (r, b_4) can be absorbed in $P_0[(r, b_1)]$ only. After this operation the node grouping P_1 still does not yield a shape graph that recognizes $\overline{G_0}$. In the next step, (r, b_3) being ctx-dominated by its sibling (r, b_4) is absorbed in $P_1[(r, b_1)]$. The resulting node grouping P_2 again fails to recognize $\overline{G_0}$. Finally, the node (s, u_1) is absorbed in $P_2[(s, e_1)]$ and the resulting node grouping P_3 yields $\overline{G_0} \div P_3 \equiv H_0$ which recognizes $\overline{G_0}$. □

The algorithm hybrid-learner is a sound inference algorithm for $\mathsf{CtxSinShEx}_0$ and analogously to sim-learner it is also complete for $\mathsf{CtxSinShEx}_0(1, *)$. The full class of context-singular shape graphs is learnable with an exhaustive exploration of the exponential search space with exponentially large characteristic graphs.

▶ **Theorem 19.** $\mathsf{CtxSinShEx}_0(1, *)$ *is learnable in polynomial time and data from simple graphs.* $\mathsf{CtxSinShEx}_0$ *is learnable from simple graphs.*

6.2 Absorption-protected shape graphs

In this section we characterize the subclass of $\mathsf{CtxSinShEx}_0$, using all basic intervals $\mathsf{M}_0 = \{1, ?, +, *\}$, for which hybrid-learner is sound and complete. To do that we first identify the information that needs to be contained in the input graph for hybrid-learner to infer the right arity on the edge of a the goal shape graph.

Let us fix a goal shape graph H and an edge $(t, a, s) \in E_H$. For hybrid-learner to output H, it must be able to construct from a characteristic graph G two groups of nodes P_t and

P_s that characterize the interval $\mathsf{arity}_H(t, a, s)$. In particular, they must contain sufficient information to indicate whether the interval is unbounded (+ and ∗) and whether it is nullable (? and ∗).

Characterizing an unbounded interval is relatively simple. It suffices to introduce in G a ctx-maximal node n_t of type t that has at least two outgoing a-edges to nodes n_s and m_s of type s, one of which, say n_s should also be ctx-maximal. Naturally, the nodes n_t and n_s will be put by hybrid-learner in the groups P_t and P_s respectively. Because of the first rule of the preference order Φ, the node m_s will also be added to P_m.

Characterizing a nullable interval is more challenging since it requires making sure that P_t and P_s absorb information that is more volatile. Namely, we need to make sure that G has a ctx-maximal node n_t and a node m_t of type t without any a-edge to a node of type s. Since n_t is ctx-maximal, it will be absorbed in P_t but since m_t is not a ctx-maximal node, G must protect it from being absorbed by any group other than P_t. The node m_t can be absorbed into a group $P_{s'}$, representing a type s', if s' dominates a version η of the type t from which we remove the edge (t, a, s). Naturally, m_t is protected if no such node exists, and then the second rule of Φ ensures that m_t ends up in P_t. Otherwise, the type t allows protection from an absorption if t has an incoming edge with unbounded arity and none of the siblings of t dominate η. Then m_t also ends up in P_t because of the first rule of Φ for same reasons as explained for unbounded intervals.

To characterize the classes of schemas that allow protection from absorption we need to introduce a construction of the type η. Formally, let H be a shape graph H, $\eta \in \mathcal{N} \setminus N_H$ a fresh node identifier, and $e \in E_H$ an edge from t to s with unbounded arity. The *absorption-protection test graph* $\mathsf{APT}^*(H, e, \eta)$ is a shape graph H' defined as:

$$N_{H'} = N_H \cup \{\eta\},\ E_{H'} = E_H \cup \{(\eta, a, s') | (t, a, s') \in \mathsf{out}_H(t) \setminus \{e\}\},\ \mathsf{arity}_{H'}(f) = * \text{ for } f \in E_{H'}.$$

Essentially, we add the type η, for every outgoing edge e' from t other than e, we add an outgoing edge with the same label as e' from η to the same node as the endpoint of e', and we set arities of all edges to ∗. Next, we formally characterize the class of shape graphs that hybrid-learner is capable of identifying (we use sim-domination because η in $\mathsf{APT}^*(H, e, \eta)$ does not have any incoming edges).

▶ **Definition 20.** *A type t of a shape graph H is* absorption-protected *iff for every edge $e \in \mathsf{out}_H(t)$ with nullable arity one of the following conditions holds:*

1. *t is the only node that sim-dominates η in $\mathsf{APT}^*(H, e, \eta)$ or,*
2. *t has an incoming edge with unbounded arity and t is the only node among its siblings that sim-dominates η in $\mathsf{APT}^*(H, e, \eta)$.*

An absorption-protected *shape graph is a context-singular shape graph that has only absorption-protected types. By $\mathsf{AbsShEx}_0$ we denote the set of all absorption-protected shape graphs.*

We illustrate absorption protection in the following example.

▶ **Example 21.** In Figure 10, H_1 is not absorption-protected because of the edge $e = (t_1, a?, \mathsf{str})$. The copy η of t_1 without the edge e is sim-dominated by the type t_2 of H_1. H_2 is absorption-protected. Even if for the type s_1 we create a copy η without the edge $(s_1, a?, \mathsf{str})$ and find it is sim-dominated by s_2, the type s_1 has an incoming unbounded r-edge and the type s_2 is not a sibling of s_1.

We point out that the shape graph in Figure 1 is absorption protected, which explains why in Example 18 the algorithm correctly infers the schema H_0. We finish by formally stating the learnability result.

▶ **Theorem 22.** $\mathsf{AbsShEx}_0$ *is learnable in polynomial time and data from simple graphs.*

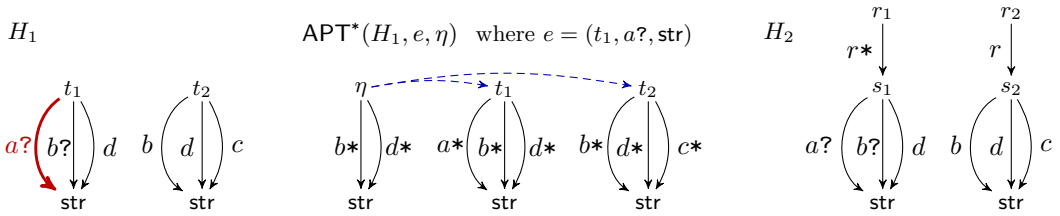


Figure 10 Two shape graphs, H_1 is not absorption-protected because t_1 is not, but H_2 is.

7 Schemas of existing graph databases

In this section we present an analysis (Table 1) of a number of graph databases in order to find out to what extent their schemas can be captured with shape graphs and the subclasses that we propose, and consequently, to assess the usefulness of the proposed inference algorithms. We have analyzed: the Berlin SPARQL Benchmark [10], the Tpc-h benchmark converted to RDF with Direct Mapping [51, 54], the Nobel Prize database [4], an RDF serialization of the Dblp database (retrieved from `https://www.rdfhdt.org/datasets/` on 14.01.2021), the Springer Nature knowledge graph SciGraph [32], the Covid19 knowledge graph [43], and SHACL constraints in the version 4 of Yago knowledge base [50]. For each database we have defined appropriate schemas using ShEx, which is a fully fledged schema language and properly contains ShEx_0 (cf. [47]). Complete schemas and more details can be found in the appendix.

	Base types						Union	Clauses		
	total	Det	σ-ind	Sin	CtxSin	Abs	types	total	union	disj.
Dblp	11	5	6	8	10	7	2 (3)	135	2 (9)	1
Berlin	8	8	5	5	8	7	0 (0)	47	0 (0)	0
Tpc-h (dm)	8	8	8	8	8	8	0 (0)	67	0 (0)	0
Nobel	11	8	7	7	10	8	1 (0)	66	2 (0)	1
SciGraph	18	10	16	17	18	16	1 (2)	162	1 (7)	1
Covid19	22	11	11	19	19	19	2 (0)	295	3 (0)	0
Yago	49	14	28	28	30	21	2 (13)	1174	4 (490)	0

Table 1 Analysis of schemas for a number of graph databases.

We have found that the ShEx schemas for the above databases require the use of *disjunction* and *union types*, features that are absent in ShEx_0 [47, 55]. We illustrate them on the following example inspired by DBLP.

$$\mathsf{Book} \to (\mathit{creator} : \mathsf{Person+} \mid \mathit{editor} : \mathsf{Person+}),\ \mathit{title} : \mathsf{Literal},\ \mathit{ref} : (\mathsf{Article} \cup \mathsf{Book})*.$$

It states that a book has either creators (authors) or editors but never both, has a single title, and references an arbitrary number of articles and books. We say that this base type definition has 3 clauses, one uses disjunction, and one uses a union type. Union types are *trivial* when used only under $*$ since $a : (t_1 \cup t_2)*$ is equivalent to $a : t_1*,\ a : t_2*$. For every schema we have measured the quantities of the following objects: nontrivial (and trivial) union types, clauses, clauses with disjunction, clauses with nontrivial (and trivial) use of a union type.

To help assessing the usefulness of the proposed inference algorithms, for every ShEx schema we have constructed its straightforward ShEx_0-approximation as illustrated on the

example for the above type definition of Book

$$\mathsf{Book} \to \mathit{creator} : \mathsf{Person}*,\ \mathit{editor} : \mathsf{Person}*,\ \mathit{title} : \mathsf{Literal},\ \mathit{ref} : \mathsf{Article}*,\ \mathit{ref} : \mathsf{Book}*.$$

Then in each ShEx_0 we have measured the number of all (base) types, those that are singular (Sin), context-singular (CtxSin), and absorption-protected (Abs). Additionally, we have counted the number of types that are signature-independent (σ-ind): types whose set of labels of outgoing edges is incomparable with others.

We first analyze our findings for the graph databases and knowledge graphs (first 6 rows). We observe that the numbers of nontrivial union types and disjunctions are relatively small. Also, deterministic types are relatively low in some databases because of use of union types: even trivial use of union types in a type definition precludes determinism. We point to the differences in signature-independent and singular types, on average 69% vs. 79% resp., which indicates that using simulation to identify types has advantages over an approach that reduces a type to the labels of its outgoing types. While the numbers of singular types are relatively large, 79% on average, the numbers of context-singular types, 94% on average, are even more impressive, and the significant improvement validates our approach of incorporating the context information in the inference process.

For the knowledge base YAGO the results indicate that our algorithms would offer little improvement over simpler approaches (σ-ind) that attempt to identify types by using the labels of their outgoing edges. We attribute this to the use of rich hierarchies of classes which introduce many subtype relationships between types. We point out, however, that those class hierarchies are defined with ontologies that specify rules that allow to type the graph. Our methods do not take advantage of this typing information, and therefore, are not geared towards inference for knowledge bases. Alternative tools for inference from typed graphs should be used (see our preliminary results on the topic in [30]).

We conclude that inference algorithms for the proposed classes $\mathsf{CtxSinShEx}_0$ and $\mathsf{AbsShEx}_0$ are an attractive choice for the first draft of the schema for (untyped) graph databases and knowledge graphs to be later on improved by a data specialist, especially when the type hierarchy is relatively flat.

8 Related work

Several approaches have been investigated in the late 90's to summarize graph data, defining schema models, and algorithms to infer schemas from graph data, then viewed as semi-structured data [15, 24, 41, 40]. A large part of the literature focuses on graph summarization [14], where the purpose is to obtain a concise representation of an input graph that can be used to formulate queries against the data. Our approach takes a different perspective of the same problem, where the input data is considered as evidence from which we must infer an unknown target schema. Using the grammatical inference framework enables us to offer strong guarantees, and lay the ground for a principled fundamental approach. To the best of our knowledge this is a first, and this complements the traditional approach in the literature that consists in evaluating algorithms empirically on real-life graph data to measure the tradeoff between compactness and the accuracy of the description.

A *Dataguide* [29] of a graph represents as a DFA all the paths that can be navigated from a root node in the graph. Dataguides are thus similar in spirit to our determinization procedure, but do not represent the arity of paths and assume that specific entry points have been specified; the root nodes. This approach, like determinization, can identify subtypes, and cycles (provided the cycles are presented in the input data). Several approaches have been proposed to infer schemas for tree-structured data [25, 39, 21, 8, 9] or JSON data [5, 6]. The

schemas inferred include DTDs, tree automata, and XML Schema, and thus are expressive enough to represent the arity of edges. However, these approaches focus on tree-structure and do not consider cycles (as expressed via mechanisms such as ID/REF). The tree structure means that the schema can be inferred recursively, and thus the task is essentially about inferring efficiently a regular expression representing for the children of each tree node.

More recently, the inference of schemas for graphs has focused on RDF and property graphs [34]. Several applications [23, 56, 33, 52] rely on graph (bi)simulation to build a quotient graph w.r.t. an equivalence relation. The quotient graph merges all nodes that belong to the same equivalence class. Those proposals generally do not assign arities to the edges with a few exceptions such as [53]. Variants [16, 44, 52] consider both forward and backward bisimilarity, which means that types can be defined based on both the incoming and outgoing edges. Full bisimulation is rather rare in heterogenous graphs and even limiting it to the 1-hop neighbourhood does not help [26, 20, 18, 27], so the authors introduce weak and strong equivalence relations that relax rather aggressively the bisimulation relation through transitive co-occurrence of edge labels, to achieve more compact graph summaries. Type hierarchies essentially collapse in summaries built on weak or strong equivalence whenever they would collapse for hybrid-learner. Actually, weak equivalence systematically collapses hierarchies (except for nodes without outgoing edges). Even these summaries may become large for big, encyclopedic graphs, such as DBPedia or YAGO. One solution they suggest is to use methods based on mining frequent patterns [19]. An alternative approach to such problematic graphs is to use semi automatic methods where the construction of schema is interactively guided by domain experts [12].

Other ideas include clustering nodes according to thresholds on the number of shared edge labels [53]. In [3] integer linear programming is used to optimize the tradeoff between the number of partitions and how well each partition fits to the schema, however, the fitness is defined using outbound neighborhood, and not the context. Finally, some approaches complement the structural information with types that may be already present in graphs [16, 27] or, in the case of property graphs, by inferring the typing from node labels [37].

Among results on grammatical inference, [31] shows that a family of well-behaved inference algorithms can be interpreted as constructing a least upper bound for the input in the lattice of languages from the class, where the order is defined as the containment of languages. Our inference algorithm follows a similar approach. It does not compute a least upper bound among the whole class of graph schemas, but rather inside the lattice of the graph aggregates of the input graph (see Section 3.3).

9 Conclusions and future work

We have presented a principled approach to the problem of inference of shape graphs, which are a subclass of shape expression schemas for graph databases. We have employed the framework of grammatical inference to identify key challenges: identifying arities on edges and identifying recursive types. To confront these challenges we have explored an approach of inferring shape graphs using simulation relation on the nodes of the input graph. This approach addresses well the identified challenges at the price of identifying subtypes, which we argue to be a fundamental limitation. To overcome it we extend the simulation based approach with a modest amount of context information. The resulting inference algorithm allows to infer a rich class of schemas, which we argue to be of practical importance with an empirical study of real-life schemas of graph databases.

Future research directions include exploring techniques for inference of disjunctions [11] and adapting the proposed methods to the emerging standard for Property Graph Schemas. We also plan to pursue the question of inference of shape graphs from typed graphs, our preliminary results are very promising [30].

References

1. S. Abiteboul, M. Arenas, P. Barceló, M. Bienvenu, D. Calvanese, C. David, R. Hull, E. Hüllermeier, B. Kimelfeld, L. Libkin, W. Martens, T. Milo, F. Murlak, F. Neven, M. Ortiz, T. Schwentick, J. Stoyanovich, J. Su, D. Suciu, V. Vianu, and K. Yi. Research directions for principles of data management (Dagstuhl Perspectives Workshop 16151). *Dagstuhl Manifestos*, 7(1):1–29, 2018.
2. D. Angluin. Inductive inference of formal languages from positive data. *Information and Control*, 45(2):117–135, 1980.
3. M. Arenas, G. I. Diaz, A. Fokoue, A. Kementsietsidis, and K. Srinivas. A principled approach to bridging the gap between graph data and their schemas. *Proceedings of the VLDB Endowment*, 7(8):601–612, 2014.
4. R. Asif and M. A. Qadir. Enhancing the Nobel Prize schema. In *International Conference on Communication, Computing and Digital Systems (C-CODE)*, pages 193–198, 2017.
5. M. A. Baazizi, H. Ben Lahmar, D. Colazzo, G. Ghelli, and C. Sartiani. Schema inference for massive JSON datasets. In *International Conference on Extending Database Technology (EDBT)*, 2017.
6. M. A. Baazizi, D. Colazzo, G. Ghelli, and C. Sartiani. Parametric schema inference for massive JSON datasets. *The VLDB Journal*, 28(4):497–521, 2019.
7. G. J. Bex, W. Gelade, F. Neven, and S. Vansummeren. Learning deterministic regular expressions for the inference of schemas from XML data. *ACM Transactions on the Web*, 4(4):1–32, 2010.
8. G. J. Bex, F. Neven, T. Schwentick, and K. Tuyls. Inference of concise DTDs from XML data. In *International Conference on Very Large Databases (VLDB)*, pages 115–126, 2006.
9. G. J. Bex, F. Neven, and S. Vansummeren. Inferring XML schema definitions from XML data. In *International Conference on Very Large Databases (VLDB)*, pages 998–1009, 2007.
10. C. Bizer and A. Schultz. The Berlin SPARQL benchmark. *International Journal on Semantic Web and Information Systems*, 5:1–24, 2009.
11. I. Boneva, R. Ciucanu, and S. Staworko. Schemas for unordered XML on a DIME. *Theory of Computing Systems*, 2014.
12. I. Boneva, J. Dusart, D. Fernández-Álvarez, and J. E. Labra Gayo. Semi automatic construction of shex and SHACL schemas. *CoRR*, abs/1907.10603, 2019. `arXiv:1907.10603`.
13. I. Boneva, J. Lozano, and S. Staworko. Relational to RDF data exchange in presence of a shape expression schema. In *Alberto Mendelzon International Workshop on Foundations of Data Management*, 2018.
14. A. Bonifati, S. Dumbrava, and H. Kondylakis. Graph summarization. *CoRR*, abs/2004.14794, 2020. `arXiv:2004.14794`.
15. P. Buneman, S. B. Davidson, M. F. Fernandez, and D. Suciu. Adding structure to unstructured data. In *International Conference on Database Theory (ICDT)*, pages 336–350, 1997.
16. S. Campinas, R. Delbru, and G. Tummarello. Efficiency and precision trade-offs in graph summary algorithms. In *International Database Engineering & Applications Symposium (IDEAS)*, pages 38–47, 2013.
17. J. Carme, R. Gilleron, A. Lemay, and J. Niehren. Interactive learning of node selecting tree transducers. *Machine Learning*, 66(1):33–67, 2007.
18. Š. Čebirić, F. Goasdoué, P. Guzewicz, and I. Manolescu. Compact summaries of rich heterogeneous graphs. Research Report RR-8920, INRIA Saclay ; Université Rennes 1, 2018.
19. Š. Čebirić, F. Goasdoué, H. Kondylakis, D. Kotzinos, I. Manolescu, G. Troullinou, and M. Zneika. Summarizing semantic graphs: a survey. *VLDB J.*, 28(3):295–327, 2019.
20. Š. Čebirić, F. Goasdoué, and I Manolescu. A framework for efficient representative summarization of RDF graphs. In *International Semantic Web Conference (ISWC)*, 2017.
21. B. Chidlovskii. Schema extraction from XML: A grammatical inference approach. In *Knowledge Representation Meets Databases (KRDB)*, volume 45, 2001.

22 R. Ciucanu and S. Staworko. Learning schemas for unordered XML. In *International Symposium on Database Programming Languages (DBPL)*, 2013.

23 W. Fan, J. Li, X. Wang, and Y. Wu. Query preserving graph compression. In *ACM SIGMOD International Conference on Management of Data*, pages 157–168, 2012.

24 M. Fernandez and D. Suciu. Optimizing regular path expressions using graph schemas. In *International Conference on Data Engineering (ICDE)*, pages 14–23, 1998.

25 M. Garofalakis, A. Gionis, R. Rastogi, S. Seshadri, and K. Shim. XTRACT: learning document type descriptors from XML document collections. *Data Mining and Knowledge Discovery*, 7(1):23–56, 2003.

26 F. Goasdoué, P. Guzewicz, and I. Manolescu. Incremental structural summarization of RDF graphs. In *International Conference on Extending Database Technology (EDBT)*, 2019.

27 F. Goasdoué, P. Guzewicz, and I. Manolescu. RDF graph summarization for first-sight structure discovery. *The VLDB Journal*, 29(5):1191–1218, 2020.

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

29 R. Goldman and J. Widom. Dataguides: Enabling query formulation and optimization in semistructured databases. In *International Conference on Very Large Data Bases (VLDB)*, pages 436–445, 1997.

30 B. Groz, A. Lemay, S. Staworko, and P. Wieczorek. Inference of shape expression schemas typed RDF graphs. *CoRR*, abs/2107.04891, 2021. `arXiv:2107.04891`.

31 J. Heinz, A. Kasprzik, and T. Kötzing. Learning in the limit with lattice-structured hypothesis spaces. *Theoretical Computer Science*, 457:111–127, 2012.

32 A. Iana, S. Jung, P. Naeser, A. Birukou, S. Hertling, and H. Paulheim. Building a conference recommender system based on SciGraph and WikiCFP. In *Semantic Systems. The Power of AI and Knowledge Graphs*, pages 117–123, 2019.

33 S. Khatchadourian and M. Consens. ExpLOD: Summary-based exploration of interlinking and RDF usage in the linked open data cloud. In *Extended Semantic Web Conference (ESWC)*, pages 272–287, 2010.

34 H. Kondylakis, D. Kotzinos, and I. Manolescu. RDF graph summarization: principles, techniques and applications. In *International Conference on Extending Database Technology (EDBT)*, pages 433–436, 2019.

35 J. E. Labra Gayo, E. Prud'hommeaux, H. Solbrig, and J. M. Alvarez Rodriguez. Validating and describing linked data portals using RDF Shape Expressions. In *Workshop on Linked Data Quality*, 2015.

36 G. Laurence, A. Lemay, J. Niehren, S. Staworko, and M. Tommasi. Learning sequential tree-to-word transducers. In *Language and Automata Theory and Applications (LATA)*, pages 490–502, 2014.

37 H. Lbath, A. Bonifati, and R. Harmer. Schema inference for property graphs. In *International Conference on Extending Database Technology (EDBT)*, pages 499–504, 2021.

38 A. Lemay, S. Maneth, and J. Niehren. A learning algorithm for top-down XML transformations. In *ACM Symposium on Principles of Database Systems (PODS)*, pages 285–296, 2010.

39 J.-K. Min, J.-Y. Ahn, and C.-W. Chung. Efficient extraction of schemas for XML documents. *Information Processing Letters*, 85(1):7–12, 2003.

40 S. Nestorov, S. Abiteboul, and R. Motwani. Extracting schema from semistructured data. In *ACM SIGMOD International Conference on Management of Data*, pages 295–306, 1998.

41 S. Nestorov, J. D. Ullman, J. L. Wiener, and S. S. Chawathe. Representative objects: Concise representations of semistructured, hierarchial data. In *International Conference on Data Engineering (ICDE)*, pages 79–90, 1997.

42 E. Prud'hommeaux, J. E. Labra Gayo, and H. Solbrig. Shape Expressions: An RDF validation and transformation language. In *International Conference on Semantic Systems*, 2015.

43 J. T. Reese, D. Unni, Callahan T. J., L. Cappelletti, V. Ravanmehr, S. Carbon, K. A. Shefchek, B. M. Good, J. P. Balhoff, T. Fontana, H. Blau, N. Matentzoglu, N. L. Harris, M. C. Munoz-Torres, M. A. Haendel, P. N. Robinson, M. P. Joachimiak, and C. J. Mungall. KG-COVID-19: A framework to produce customized knowledge graphs for COVID-19 response. *Patterns*, 2(1):100155, 2021.

44 A. Schätzle, A. Neu, G. Lausen, and M. Przyjaciel-Zablocki. Large-scale bisimulation of RDF graphs. In *Workshop on Semantic Web Information Management (SWIM)*, pages 1–8, 2013.

45 J. Sequeda, S. H. Tirmizi, Ó. Corcho, and D. P. Miranker. Survey of directly mapping SQL databases to the Semantic Web. *Knowledge Engineering Review*, 26(4):445–486, 2011.

46 J. F. Sequeda, M. Arenas, and D. P. Miranker. On directly mapping relational databases to RDF and OWL. In *International Conference on World Wide Web (WWW)*, pages 649–658, 2012.

47 S. Staworko, I. Boneva, J. E. Labra Gayo, S. Hym, E. G. Prud'hommeaux, and H. Solbrig. Complexity and expressiveness of ShEx for RDF. In *International Conference on Database Theory (ICDT)*, pages 195–211, 2015.

48 S. Staworko and P. Wieczorek. Learning twig and path queries. In *International Conference on Database Theory (ICDT)*, pages 140–154, 2012.

49 S. Staworko and P. Wieczorek. Containment of shape expression schemas for RDF. In *ACM Symposium on Principles of Database Systems (PODS)*, pages 303–319, 2019.

50 F. M. Suchanek, G. Kasneci, and G. Weikum. Yago: A core of semantic knowledge. In *International Conference on World Wide Web (WWW)*, pages 697—-0706. Association for Computing Machinery, 2007.

51 TPC. TPC benchmarks. URL: `http://www.tpc.org/`.

52 T. Tran, G. Ladwig, and S. Rudolph. Managing structured and semistructured RDF data using structure indexes. *Transactions on Knowledge and Data Engineering*, 25(9):2076–2089, 2013.

53 Y. Tsuboi and N. Suzuki. An algorithm for extracting shape expression schemas from graphs. In *ACM Symposium on Document Engineering (DocEng)*, pages 1–4, 2019.

54 W3C. A direct mapping of relational data to RDF, 2012. URL: `http://www.w3.org/TR/rdb-direct-mapping/`.

55 W3C. Shape expressions schemas, 2013. URL: `http://www.w3.org/2013/ShEx/Primer`.

56 H. Zhang, Y. Duan, X. Yuan, and Y. Zhang. Assg: adaptive structural summary for RDF graph data. In *International Semantic Web Conference (ISWC) Posters & Demonstrations Track*, pages 233–236, 2014.