Shape Expression Schemas for RDF

Semantics, Complexity, and Inference

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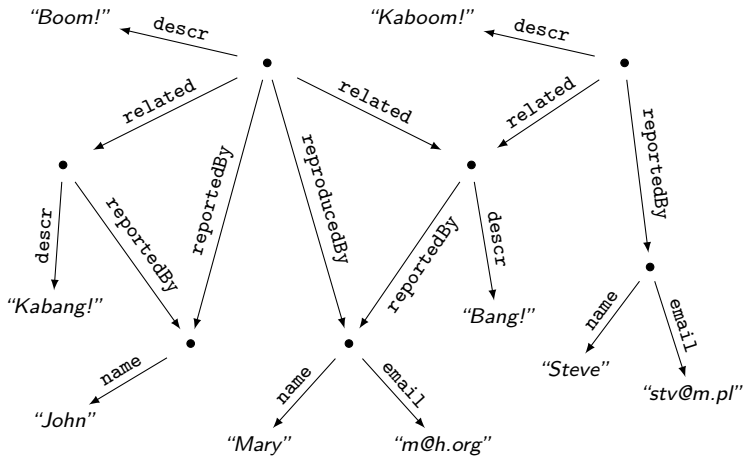
GT-ALGA 2019

Paris, France

10 October 2019

What is RDF and does it need schemas?



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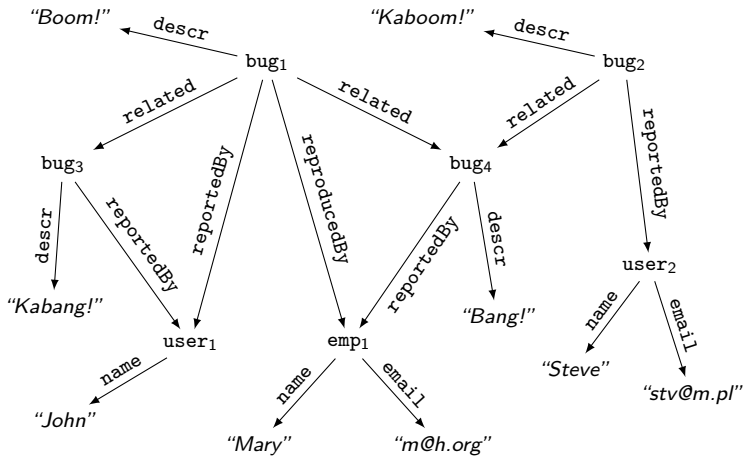


RDF at its conception and RDF now

What is RDF?

- set of triples ⟨subject, predicate, object⟩

Originally, free-range RDF

- The *driving* technology of Web 3.0 [Tim Berners-Lee]
- *"Just publish your data so others can access it!"*
- Intentionally schema-free and ontology oriented

Nowadays, industrial-strength RDF

- Produced and consumed by applications (data exchange format)
- Often obtained from exporting data from relational databases (e.g., R2RML)
- Follows a strict structure

Outline

Uses for schemas

- Provide a semantic insight into data
- Capture the structure of the graph (summary)
- Enable validation i.e., checking data conformance

If RDF that does not come with schema?

- Infer the schema

If the RDF does not satisfy its schema?

- Repair the RDF

Initial research [ICDT'15]

- Define the semantics of ShEx
- Complexity of validation
- Expressive power

Joint work with joint work with I. Boneva, J. Labra Gayo, S. Hym, E. G. Prud'hommeaux, and H. Solbrig

Current research

- Containment problem [PODS'19]
- Grammatical inference (ongoing)

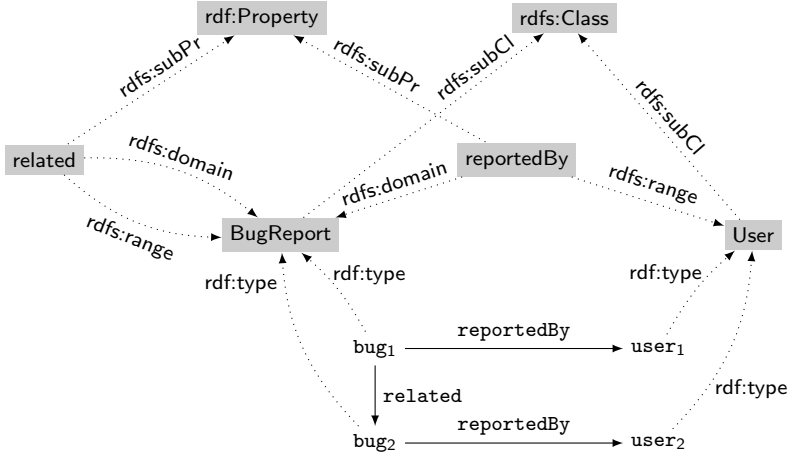
Joint work with P. Wieczorek, A. Lemay, and B. Groz

Future research

Previously existing schema formalisms for RDF

RDF Schema (RDFS) [W3C]:

- lightweight ontology language (types and type inclusion relations)
- range and domain constraints for properties (predicate types)
- virtually no power to constrain the structure of the graph



Previously existing schema formalisms for RDF (cont'd.)

OWL + CWA + UNA [Sirin, RR'10]

- Potentially confusing nonstandard semantics
- Potentially high complexity of validation

SPARQL (SPIN) [Bolleman et al., SWAT4LS'12]

- Very powerful and expressive
- High complexity

Resource Shapes [IBM, Ryman et al., LDOW'13]

- Extends RDFS with simple cardinality constraints on the outbound neighborhood of a node

What does exactly RDF validation mean

Verification the typing is given (with rdf:type) and its correctness is to be verified
(this meaning is employed by the above schema proposals)

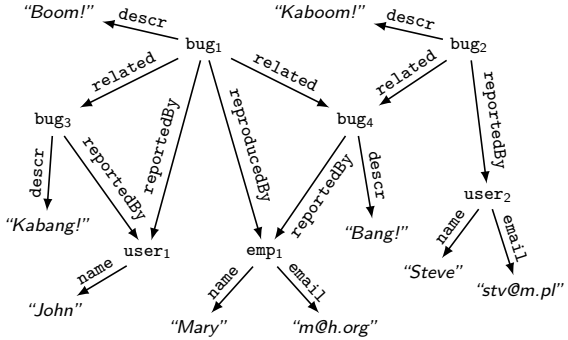
Model checking no typing is given and the goal is to construct a valid typing
(this is a more general problem that we are interested in)

Shape Expressions Schemas

Shape Expression Schema (ShEx)

Syntax

ShEx is a set of rules of the form $Type \rightarrow RegExp(Predicate \times Type)$



Bug → descr :: str,
reportedBy :: User,
reproducedBy :: Employee?,
related :: Bug*

User → name :: str,
email :: str?

Employee → name :: str,
email :: str

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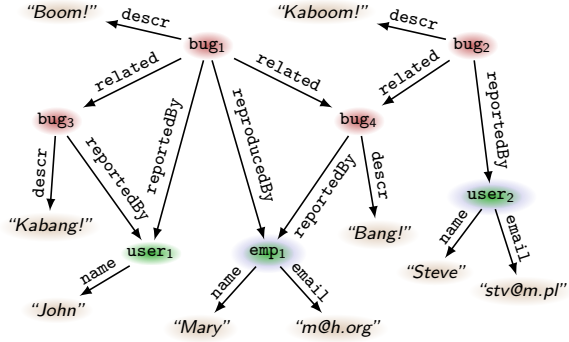



```
Bug → descr :: str,
      reportedBy :: User,
      reproducedBy :: Employee?,
      related :: Bug*
User → name :: str,
       email :: str?
Employee → name :: str,
           email :: str
```

Semantics

Graph satisfies a schema if every node has at least one type

Background information

Shape Expressions Schemas (ShEx)

- Inspired by XML Schema and reminiscent of (tree) automata
- Based on regular expressions under commutative closure
  membership NP-c [Kopczynski&To'10]; containment coNEXP-c [Haase&Hofman'16]
- Envisioned as a potential XSLT-like transformation engine for RDF

ShEx vs SHACL

- ShEx is a schema language with a growing base of users and a host of applications (e.g., Wikidata)
- SHACL is Shape Constraint Language (e.g., path constraints)
- significant overlap (upcoming paper) but also differences (recursion, negation etc.)
- comparable validation complexity (NP-complete)
- both have been developed under the tutelage of W3C
- SHACL ended up a W3C Recommendation (yay!), ShEx a W3C Community Group Project

Flavorful ShEx

```
<Emp> {
   name xsd:string | (first-name xsd:string, last-name xsd:string),
   email xsd:string,
   department @<Dept>
}

<Dept> {
   name xsd:string,
   reportedBy @<User>,
   reportedOn xsd:dateTime,
   (manager @<Emp>, appointedOn xsd:dateTime)?,
   employees @<Emp>*
}
```

Bags of symbols (unordered words)

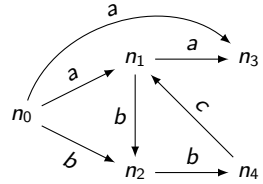
Bag (multiset) is a function mapping a symbol to the number of its occurrences.

$w_0 = \{\!|a, a, a, c, c|\!\}$ represents the function $w_0(a) = 3$, $w_0(b) = 0$, and $w_0(c) = 2$.

The collection of outgoing labels is a bag:

$$\mathit{out\text{-}lab}_G(n) = \{\!|a \mid (n, a, m) \in E_G|\!\}$$

G_0:



$\mathit{out\text{-}lab}_{G_0}(n_0) = \{\!|a, a, b|\!\}$

Bag union: $\{\!|a, c, c|\!\} \uplus \{\!|a, b|\!\} = \{\!|a, a, b, c, c|\!\}$ (concatenation of unordered words).

Regular Bag Expressions (RBEs)

Language of regular expressions for defining bags (unordered concatenation ,)

$$E ::= \epsilon \mid a \mid E^* \mid (E \text{“|”} E) \mid (E \text{“, ”} E)$$

with natural macros: $E? := (\epsilon \mid E)$ and $E^+ := (E, E^*)$

Examples

- (a^*, b^+, c, c) – arbitrary number of a's, positive number of b's, and two c's
- $(a, b)^*$ – the same number of a's and b's
- $(a, b, c)^*$ – the same number of a's, b's, and c's.

RBEs are equivalent to

1. Presburger arythmetic (PA),
2. Parikh images of context-free languages,
3. semilinear sets.

Computational properties

- Membership $w \in E$ is NP-complete,
- Emptiness $E_1 \cap E_2 = \emptyset$ is coNP-complete.

RBE_0 and $\mathrm{ShEx}_0 = \mathrm{ShEx}(\mathrm{RBE}_0)$

RBE_0

- RBEs using only symbols with multiplicities $\{0, 1, *, +, ?\}$ and , operator only
- can be canonized a, $a^? \equiv a^{[1,2]}$, b^+, $b^+ \equiv b^{[2,\infty]}$, etc.
- the canonical form is $a^{[n,n']}$, $b^{[m,m']}$, ...
- Presburger formulas: conjunctions of atoms $\#a < n$ and $\#a > n$
- captures IBM's Resource Shapes

Computational properties: simple arithmetic

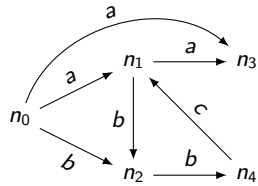
A lightweight class enjoying tractability of a number of problems:

- membership
- containment
- intersection (also with RBE_1)

Also learnable from positive examples [DBPL'13]

Getting the semantics of ShEx right

$$
\begin{aligned}
S_0\colon\quad & t_0 \to (a :: t_1)^+,\ b :: t_2 \\
& t_1 \to (a :: t_1 \mid b :: t_2)^* \\
& t_2 \to b :: t_2 \mid c :: t_1
\end{aligned}
\qquad G_0\colon
$$



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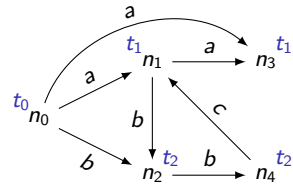

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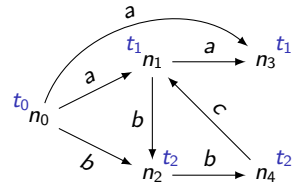


A single-type typing is a function $\lambda : V \to \Gamma$.

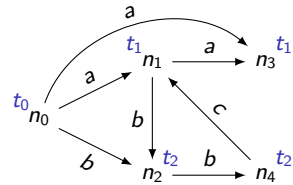
λ is valid if every node n satisfies its type definition i.e.,

$$\mathit{out\text{-}lab\text{-}type}^{\lambda}_{G}(n) = \{\!\{a :: \lambda(m) \mid (n, a, m) \in E\}\!\} \in \delta(\lambda(n)).$$

Getting the semantics of ShEx right

$$S_0: \quad t_0 \to (a :: t_1)^+,\ b :: t_2 \qquad t_1 \to (a :: t_1 \mid b :: t_2)^* \qquad t_2 \to b :: t_2 \mid c :: t_1$$

G_0:



$$\mathit{out\text{-}lab\text{-}type}^{\lambda_0}_{G_0}(n_0) = \{\!|a :: t_1, a :: t_1, b :: t_2|\!\}$$

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A valid single-type typing of G_0 w.r.t. S_0

$$\lambda_0(n_0) = t_0, \qquad \lambda_0(n_1) = t_1, \qquad \lambda_0(n_2) = t_2, \qquad \lambda_0(n_3) = t_1, \qquad \lambda_0(n_4) = t_2.$$

Intractability of single-type validation

Validation problem

Checking if there exists a valid typing of given input graph w.r.t. a given input schema.

Sources of complexity

1. guessing a typing
2. checking that it is valid (RBE membership is already NP-complete)

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Theorem

Single-type validation is NP-complete (even if only RBE_0 *are used).*

Reduction from graph 3-colorability:

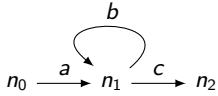
$$t_r \to \_ :: t_b^*,\ \_ :: t_g^* \qquad t_g \to \_ :: t_r^*,\ \_ :: t_b^* \qquad t_b \to \_ :: t_g^*,\ \_ :: t_r^*$$

Multi-type semantics of shape expressions

A multi-type typing is a function $\lambda : V \to 2^{\Gamma}$ that assign to every node a set of types.

S_1: $t_0 \to a :: t_1$
$t_1 \to b :: t_2,\ c :: t_3$
$t_2 \to (b :: t_2)^?,\ c :: t_3$
$t_3 \to \epsilon$

G_1:



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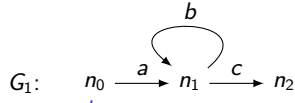

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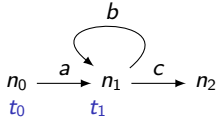

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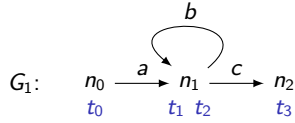

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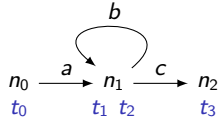

$$\lambda_1(n_0) = \{t_0\}, \qquad \lambda_1(n_1) = \{t_1, t_2\}, \qquad \lambda_1(n_2) = \{t_3\}.$$

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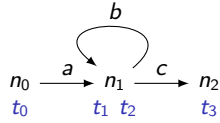

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λ is valid if every node satisfies every of its associated types.

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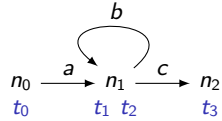

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When defining that a node n satisfies a type t...

- we inspect the outbound neighborhood $\mathit{out\text{-}lab\text{-}node}_G(n) = \{(a, m) \mid (n, a, m) \in E\}$

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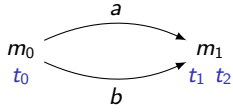
$$S_2: \quad t_0 \to a :: t_1,\ b :: t_2$$
$$t_1 \to (c :: t_1)^*$$
$$t_2 \to (d :: t_2)?$$

G_2:



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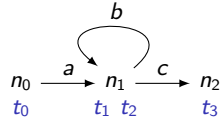

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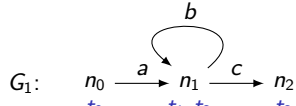

$OutType(n_1, \lambda_1) = (b :: t_1 \mid b :: t_2),\ c :: t_3$

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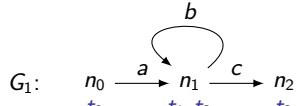

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n satisfies t w.r.t. λ if $OutType(n, \lambda) \cap \delta(t) \neq \emptyset$,
where $OutType(n, \lambda) = \bigcirc_{(n,a,m)\in E}(|_{t\in\lambda(m)}\ a :: t)$

Refinement algorithm

The set of all valid multi-type typings of G w.r.t. S is a semi-lattice.

1. Start with the universal typing $\lambda(n) := \Gamma$
2. Iteratively refine it $\lambda := \mathit{Refine}(\lambda)$

$$[\mathit{Refine}(\lambda)](n) = \{t \in \lambda(n) \mid \mathit{OutType}(n, \lambda) \cap \delta(t) \neq \emptyset\}.$$

3. Until a fix-point is reached
4. The graph satisfies the schema iff the fix-point λ is valid ...
   ... and then λ is also the maximal valid multi-type typing.

Satisfiability of RBEs

OutType yields expressions of the form (RBE_1)

$$(a_1 \mid \cdots \mid a_k),\ \cdots,\ (z_1 \mid \ldots \mid z_m)$$

The essential decision problem for a class $\mathcal{C}$ of RBEs used in the ShEx schema is

$$\mathrm{INTER}_1(\mathcal{C}) = \{(E_0, E) \in \mathrm{RBE}_1 \times \mathcal{C} \mid E_0 \cap E \neq \emptyset\}.$$

Lemma
Tractability of INTER_1 *is a necessary and sufficient condition for tractability of multi-type validation.*

Corollary
Multi-type validation is NP-complete.

Theorem
Multi-type validation for $\mathrm{ShEx}_0 = \mathrm{ShEx}(\mathrm{RBE}_0)$ *is in PTIME*

Determinism

Determinism of shape expressions

Given the type (of a node) and the label of an outgoing edge, the expression specifies the type that the target node must satisfy.

$a :: t_1,\ b :: t_2^*,\ a :: t_1,\ c :: t_2$ deterministic

$(a :: t_1,\ b :: t_2) \mid (a :: t_3,\ c :: t_4)$ not deterministic

$a :: t_1,\ b :: t_2^*,\ a :: t_3$ not deterministic

Determinism

Determinism of shape expressions

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$a :: t_1,\ b :: t_2^*,\ a :: t_1,\ c :: t_2$ $\quad$ $(a :: t_1,\ b :: t_2) \mid (a :: t_3,\ c :: t_4)$ $\quad$ $a :: t_1,\ b :: t_2^*,\ a :: t_3$

deterministic $\quad$ not deterministic $\quad$ not deterministic

Lemma

For schemas using only deterministic shape expressions, tractability of membership is a sufficient and necessary condition for tractability of multi-type validation

Proof sketch

- Knowing the label a of an outgoing edge determines the type t_a for the target node
- $\mathit{OutType}(n, \lambda) = \textcircled{,}_{(n,a,m)\in E}(|_{t\in\lambda(m)}\ a :: t)$ becomes $\textcircled{,}_{(n,a,m)\in E}(a :: t_a)$
- $\textcircled{,}_{(n,a,m)\in E}(a :: t_a)$ defines a singleton $\{w\}$ with $w = \{\!|a :: t_a \mid (n, a, m)|\!\}$
- $\mathit{OutType}(n, \lambda) \cap \delta(t) \neq \emptyset \equiv w \in \delta(t)$.

Single-occurrence REBs (SORBEs)

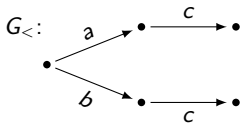
SORBE allows a symbol to be used at most once in an expression but also allows $a^{[n,m]}$

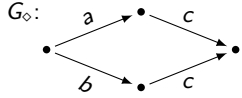
Theorem
Membership for SORBE is in PTIME :)

$a :: t_1,\ b :: t_2^*,\ a :: t_1$	$(a :: t_1,\ b :: t_2) \mid (a :: t_3,\ c :: t_4)$	$(a :: t_1,\ b :: t_2)^*,\ c :: t_3$
deterministic but not single-occurrence	not deterministic yet single-occurence	deterministic and single-occurrence

Theorem
Multi-type validation for deterministic shape expressions using SORBE *is in PTIME. :)*

Expressive power of ShEx





	FO_G	$ShEx_m$	$ShEx_s$	$\exists MSO_G$
$L : G_\diamond \in L,\ G_< \in L$	✓	✓	✓	✓
$L : G_\diamond \notin L,\ G_< \in L$	✓	×	✓	✓
$L : G_\diamond \in L,\ G_< \notin L$	✓	×	×	✓

Quick recap

Complexity

	RBE_0	RBE	SORBE	SORBE det.
multi-type	PTIME	NP-complete		PTIME
single-type	NP-complete			

Expressive power

- automata-like formalism
- incomparable with FO and MSO (unless we forbid $*$ over expressions)
- captured with MSO+PA
- incomparable with NR and HR graph grammars
- closed under intersection but not under union or negation
- single-type semantics is more expressive than multi-type semantics

Containment of ShEx

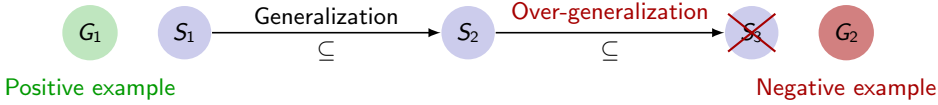
Containment problem

Containment $S_1 \subseteq S_2$

Does every graph that satisfies S_1 also satisfies S_2?

Motivation

- Fundamental problem (static analysis: query optimization, schema minimization etc.)
- Inference of ShEx (work in progress)

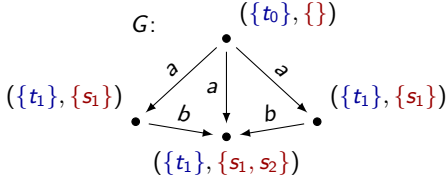


The challenge

- RBEs = Presburger Arithmetic (PA)
- $\text{MSO}_\text{G} \not\supseteq \text{ShEx} \subseteq \text{MSO}_\text{G} + \text{PA}$
- MSO_G with very little arithmetic becomes undecidable [Elgot&Rabin'66]

Decidability of Containment

$$S_1: \quad t_0 \to a :: t_1^* \qquad t_1 \to b :: t_1^? \qquad \not\subseteq \qquad S_2: \quad s_0 \to a :: s_1 \mid (a :: s_1,\ a :: s_2)^* \qquad s_1 \to b :: s_2^? \qquad s_2 \to \epsilon$$



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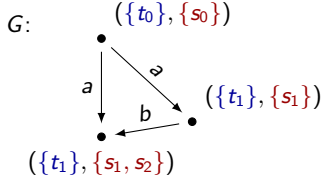

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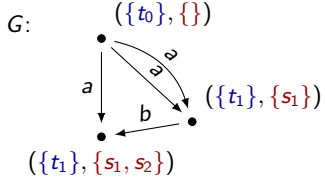

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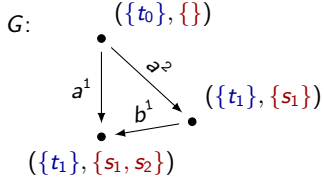

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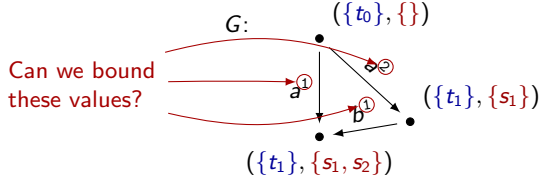

Containment of ShEx is in co2NEXP$^{\text{NP}}$

- The counter-example is a graph with at most exponential number of nodes, one node per (A, B)-kind
- There is a PA formula φ that describes the multiplicities
- PA enjoys an upper bound $O(|\varphi|^{3|\bar{x}|^k})$ on minimal solutions [Weispfenning'90]
- Double exponential upper bound on the (binary) size of the values of multiplicities
- Validation of graphs with multiplicities remains in NP

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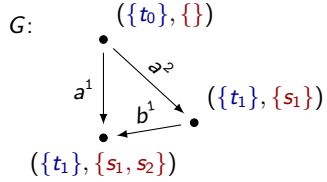
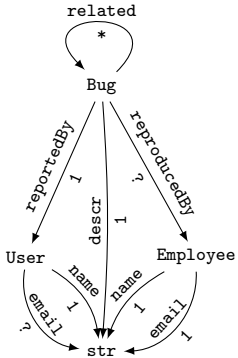


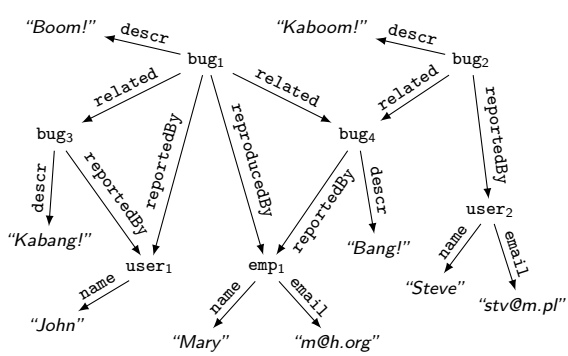
Containment of ShEx is in co2NEXP^{NP} and coNEXP-hard

- The counter-example is a graph with at most exponential number of nodes, one node per (A, B)-kind
- There is a PA formula φ that describes the multiplicities
- PA enjoys an upper bound $O(|\varphi|^{3|\bar{x}|^k})$ on minimal solutions [Weispfenning'90]
- Double exponential upper bound on the (binary) size of the values of multiplicities
- Validation of graphs with multiplicities remains in NP
- Containment of commutative REs recently shown to be coNEXP-hard [Haase&Hofman'16]

ShEx_0

- no disjunction $(a :: t_1 \mid b :: t_2)$ and no grouping $(a :: t_1, b :: t_2)^*$
- Shape Graphs – an equivalent graphical representation





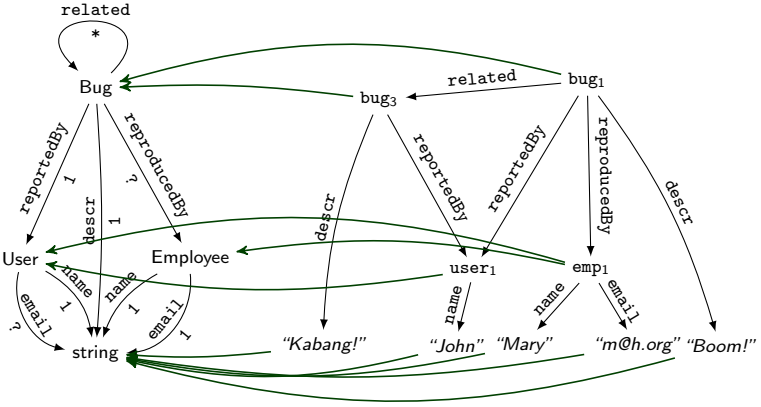
$\texttt{Bug} \rightarrow \texttt{descr} :: \texttt{str},\ \texttt{reportedBy} :: \texttt{User},\ \texttt{reproducedBy} :: \texttt{Employee}^?,\ \texttt{related} :: \texttt{Bug}^*$

$\texttt{User} \rightarrow \texttt{name} :: \texttt{str},\ \texttt{email} :: \texttt{str}^?$

$\texttt{Employee} \rightarrow \texttt{name} :: \texttt{str},\ \texttt{email} :: \texttt{str}$

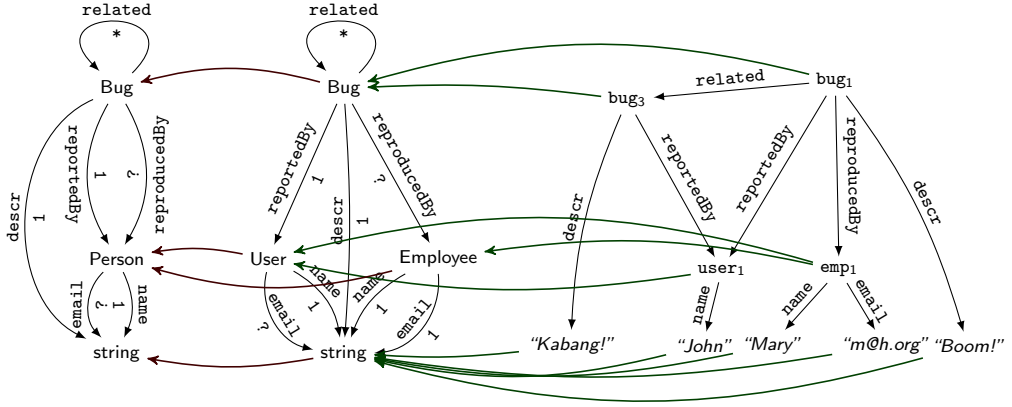
Embeddings

- Graph morphism with occurrence constraints, closely related to graph simulations
- Capture semantics of ShEx_0 by means of structural comparison



Embeddings

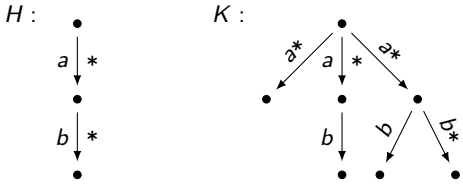
- Graph morphism with occurrence constraints, closely related to graph simulations
- Capture semantics of ShEx$_0$ by means of structural comparison
- Generalize naturally to pairs of shape graphs



Properties of embeddings

Embedding and containment

- Embedding implies containment
- In general, the converse does not hold



H cannot be embedded into K ($b :: t^*$ is equivalent to $\epsilon \mid b :: t \mid b :: t^+$)

Theorem

Constructing embeddings is

- in PTIME if only 1, ?, *, + are used
- NP-complete if arbitrary occurrence constraints are allowed $a :: t^{[n;m]}$

When does containment implies embedding?

Determinism

- DetShEx$_0$ every type uses each predicate symbol at most once
- DetShEx$_0^-$ no + are allowed and ? must be dominated by $*$

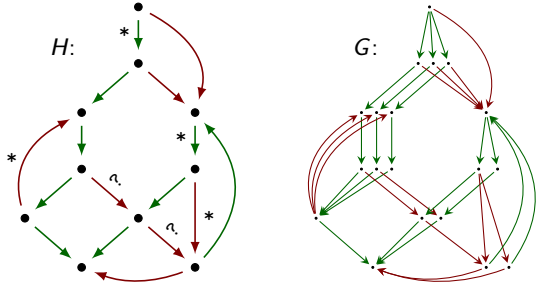
Characterizing graph

For any $H \in$ DetShEx$_0^-$ there is a polynomially-sized graph G characterizing H under containment i.e.,

$$\forall K \in \text{DetShEx}_0^-.\ G \text{ satisfies } K \Rightarrow H \subseteq K.$$

Theorem
Containment for DetShEx$_0^-$ is in PTIME

Theorem
Containment for DetShEx$_0$ is coNP-hard



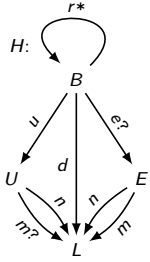
Two equivalent ShEx_0 schemas and their shape graphs

H :

$\texttt{Bug} \to \texttt{descr} :: \texttt{str},\ \texttt{reportedBy} :: \texttt{User},\ \texttt{reproducedBy} :: \texttt{Employee}^{?},$
$\texttt{related} :: \texttt{Bug}^{*}$

$\texttt{User} \to \texttt{name} :: \texttt{str},\ \texttt{email} :: \texttt{str}^{?}$

$\texttt{Employee} \to \texttt{name} :: \texttt{str},\ \texttt{email} :: \texttt{str}$



K :

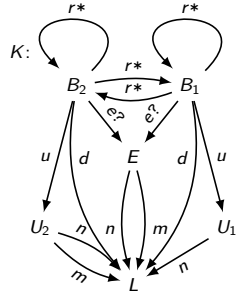
$\texttt{User}_1 \to \texttt{name} :: \texttt{str}$

$\texttt{User}_2 \to \texttt{name} :: \texttt{str},\ \texttt{email} :: \texttt{str}$

$\texttt{Bug}_1 \to \texttt{descr} :: \texttt{str},\ \texttt{reportedBy} :: \texttt{User}_1,\ \texttt{reproducedBy} :: \texttt{Employee}^{?},$
$\texttt{related} :: \texttt{Bug}_1^{*},\ \texttt{related} :: \texttt{Bug}_2^{*}$

$\texttt{Bug}_2 \to \texttt{descr} :: \texttt{str},\ \texttt{reportedBy} :: \texttt{User}_2,\ \texttt{reproducedBy} :: \texttt{Employee}^{?},$
$\texttt{related} :: \texttt{Bug}_1^{*},\ \texttt{related} :: \texttt{Bug}_2^{*}$

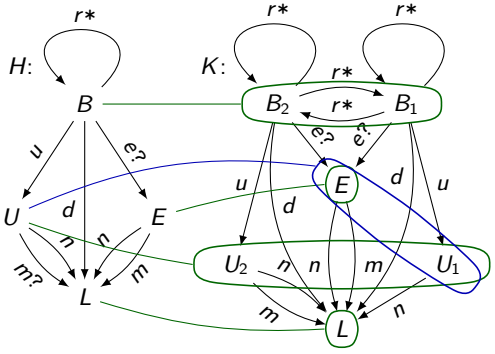
$\texttt{Employee} \to \texttt{name} :: \texttt{str},\ \texttt{email} :: \texttt{str}$



Coverings

Generalization of embeddings

A type t is covered by a set of types $S = \{s_1, \ldots, s_k\}$ iff any node satisfying t also satisfies one of the types in S

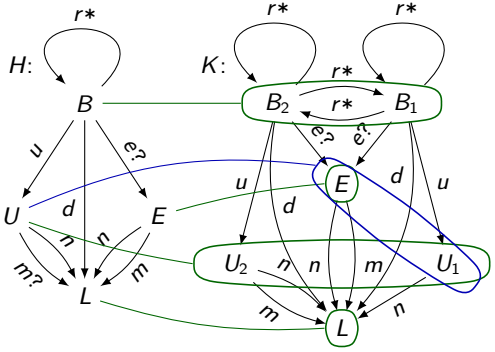


Lemma (Constructing covering)

Covering is the maximum relation $R \subseteq \text{Types}(H) \times \mathcal{P}(\text{Types}(K))$ such that

$$\forall (t, S) \in R.\ \text{def}(t) \xrightarrow{\textit{Unfold}}_R \{\text{def}(s) \mid s \in S\}.$$

Unfolding



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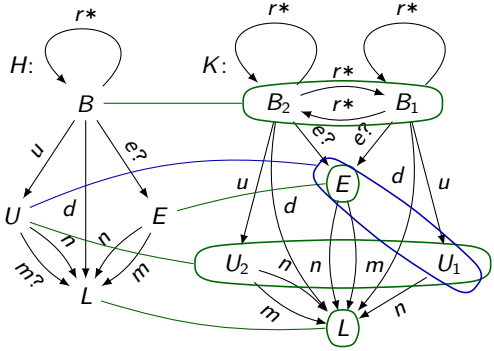
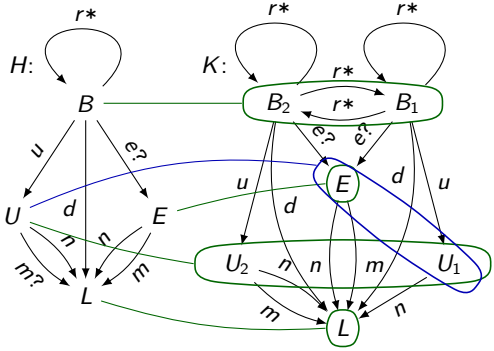


Unfolding U into $\{U_1, U_2\}$

$$U \to n :: L,\ m :: L^{?} \equiv n :: L,\ (\epsilon \mid m :: L) \equiv (n :: L) \mid (n :: L,\ m :: L) \leftarrow U_1 \mid U_2$$

Unfolding



Unfolding B into $\{B_1, B_2\}$

$$
\begin{aligned}
B &\rightarrow r :: B^*,\ u :: U,\ d :: L,\ e :: E^? \\
&\equiv (r :: B^*,\ u :: U_1,\ d :: L,\ e :: E^?) \mid (r :: B^*,\ u :: U_2,\ d :: L,\ e :: E^?) \\
&\equiv (r :: B_1^*,\ r :: B_2^*,\ u :: U_1,\ d :: L,\ e :: E^?) \mid (r :: B_1^*,\ r :: B_2^*,\ u :: U_2,\ d :: L,\ e :: E^?) \\
&\leftarrow B_1 \mid B_2
\end{aligned}
$$

Complexity of $ShEx_0$

Theorem
Containment for $ShEx_0$ is in EXP

- Covering is a relation of exponential size
- Covering can be obtained with an iterative refinement process
  (starting with maximal relation and remove at least one element at each iteration until stabilization)
- At each step unfoldings are constructed and each unfolding is a tree whose size is bounded exponentially

Theorem
Containment for $ShEx_0$ is EXP-complete

- Reduction from containment for binary tree automata

Quick recap

- Containment for ShEx is decidable
- There is a (arguably practical) class DetShEx$_0^-$ with tractable containment
- ShEx is very different from tree automata and requires novel techniques

ShEx	DetShEx	ShEx$_0$	DetShEx$_0$	DetShEx$_0^-$
coNEXP-h and co2EXP^{NP}	co2EXP	EXP-c	coNP-h	PTIME

Inference of ShEx

Constructing ShEx from an RDF Graph

What for?

- RDF originally schema-free but schemas are useful
- Free-range RDF is dirty
- Industrial-strength RDF is relatively clean and exhibits regular structure

$$\text{Relational database} \xrightarrow{\text{R2RDF}} \text{RDF}$$

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What do we want?

For a given RDF Graph G construct a ShEx schema S that captures the structure of G:

Soundness	G satisfies S
Succinctness	S is small enough for a human user to consume
Specificity	S is not overly general (as the universal schema is)

Implicit node similarity

Two nodes should have the same type if they are similar in some way. Two possible criteria:

- content – the outbound neighborhood is similar
- context – the inbound neighborhood is similar

Inference and Fitting

Fitting

For a input G construct $\subseteq$-minimal schema S that G satisfies.

Inference

An inference algorithm A is an algorithm that is

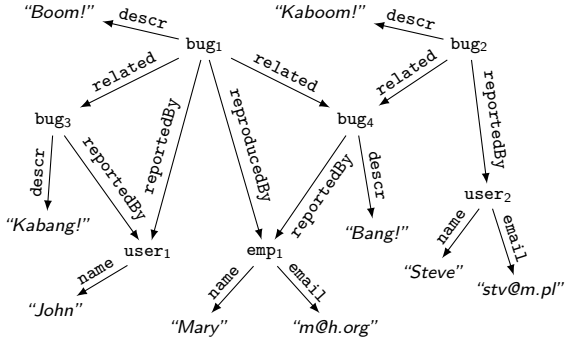
- sound i.e., it returns a schema that the input graph satisfies;
- complete i.e., it can return any goal schema provided that the input graph is sufficiently informative (or rich enough).

Both approaches are parameterized by a class $\mathcal{C}$ of goal ShEx schemas.

Bad news for Fitting: Overfitting

Fitting for ShEx_0 is trivial and potentially too verbose

An RDF graph interpreted as a shape graph is its own ShEx_0 fitting



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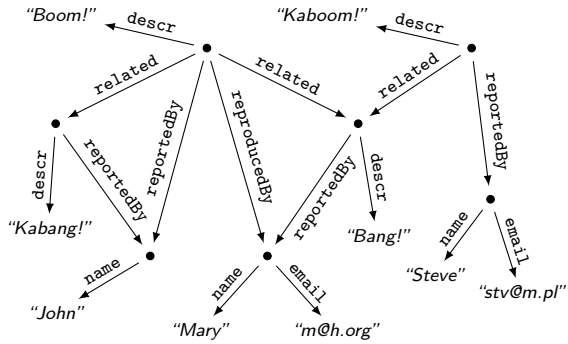

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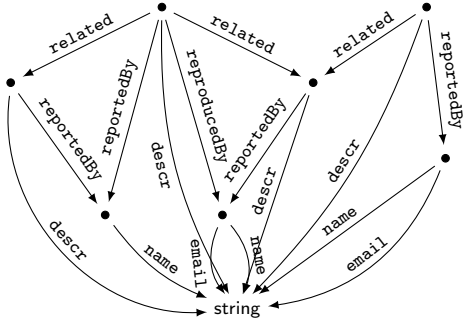

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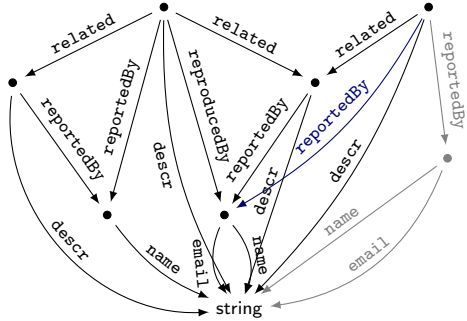


Bisimulation can identify redundant/repetitive information

But it won't generalize the result (it won't introduce $*$ or recursion).

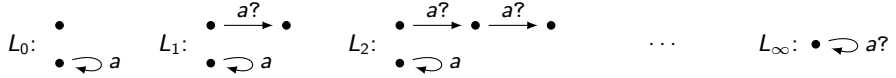
Bad news for Inference: Limit Point

Limit point

A class of languages $\mathcal{C}$ has the *limit point* property iff $\mathcal{C}$ contains an ascending chain of languages $L_1 \subsetneq L_2 \subsetneq \dots$ whose limit point $L_\infty = \bigcup_i L_i$ also belongs to $\mathcal{C}$.

Folklore result: Limit point precludes inference

No family with limit point property has an inference algorithm.



Lemma

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

So... What do we do?

We compromise

- Find a suitable subclass that allows inference and remains relatively practical.
- Motivation: first draft of a ShEx schema for an architect to work on.

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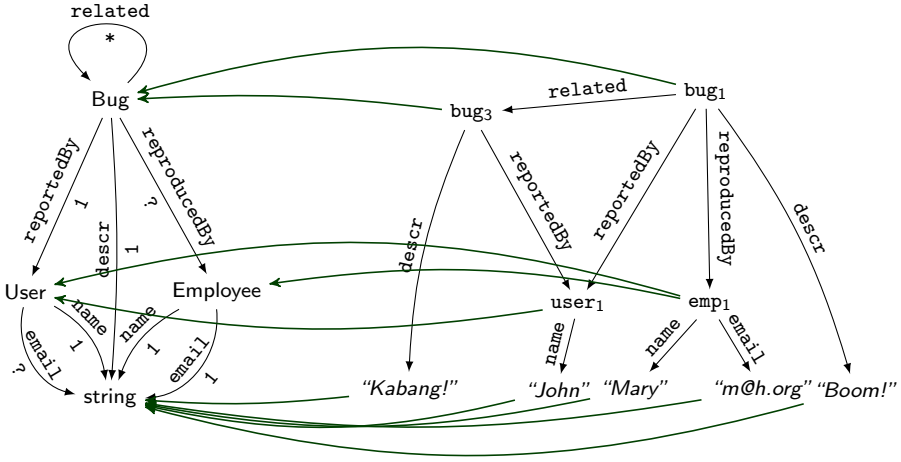
Our results

	ShEx_0	$\mathrm{SingShEx}_0$	$\mathrm{DetShEx}_0$	Typed graph
Fitting	trivial	undefined (?)	exponential	NP-hard
Inference	unfeasible	$\mathrm{SingShEx}_0(1, *)$	$\mathrm{DetShEx}_0^-$	ShEx_0 (?)

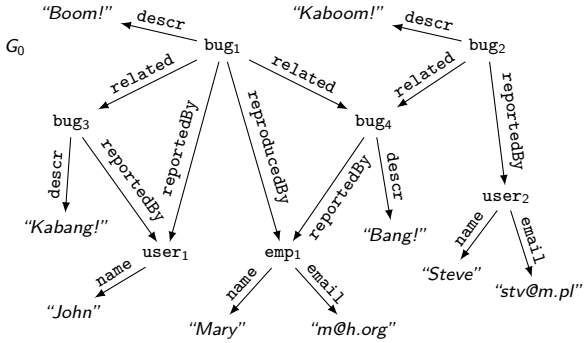
Embeddings (recall)

- Generalize simulations
- Capture semantics of ShEx by means of structural comparison

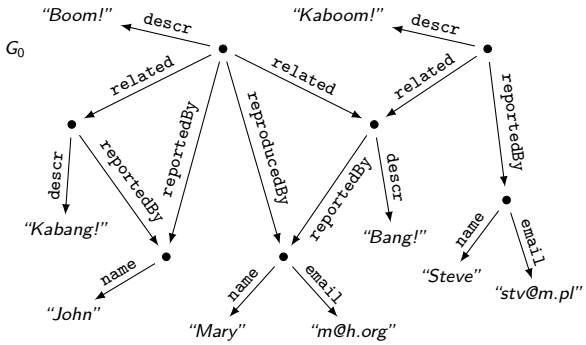


Singular Shape Expression Schemas

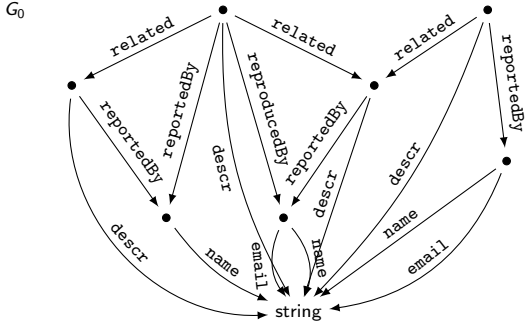
Inference of SingShEx$_0$: Generalization



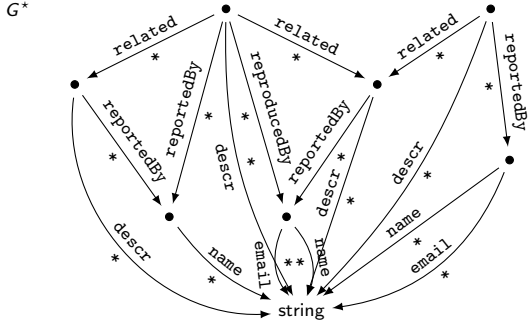
Inference of SingShEx$_0$: Generalization



Inference of SingShEx$_0$: Generalization

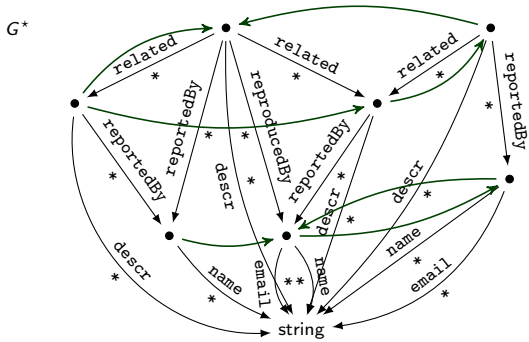


Inference of SingShEx$_0$: Generalization



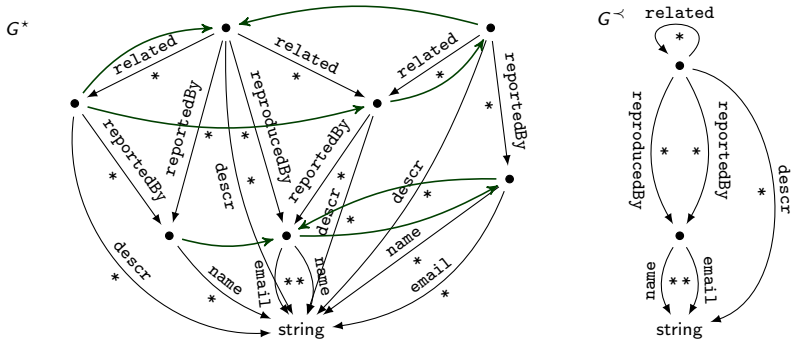
1. Put $*$ on every edge of the input graph

Inference of SingShEx$_0$: Reduction



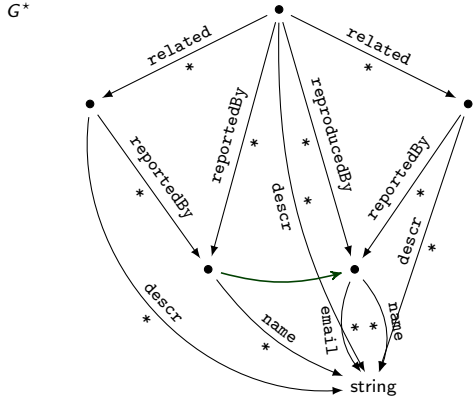
1. Put $*$ on every edge of the input graph
2. Construct the autoembedding

Inference of SingShEx$_0$: Reduction



1. Put $*$ on every edge of the input graph
2. Construct the autoembedding
3. Remove any dominated nodes

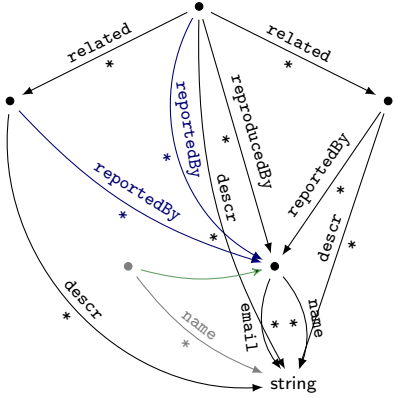
Inference of SingShEx$_0$: Reduction in detail



Removing a node n dominated by m

- remove n and all of its outgoing edges
- redirect its incoming edges to m

Inference of SingShEx$_0$: Reduction in detail



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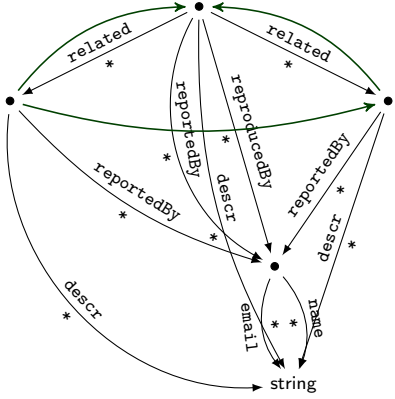

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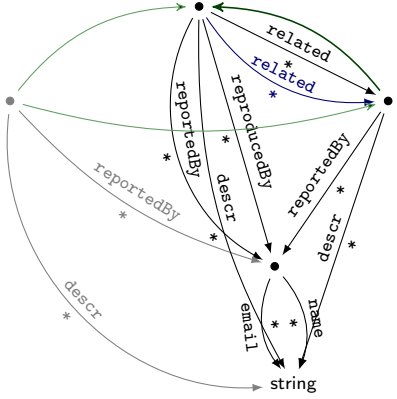
Inference of SingShEx$_0$: Reduction in detail



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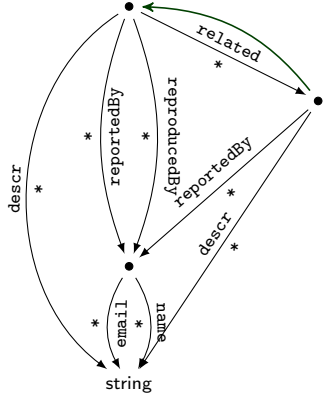

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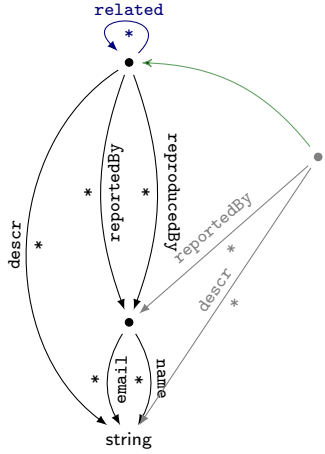
Inference of SingShEx$_0$: Reduction in detail

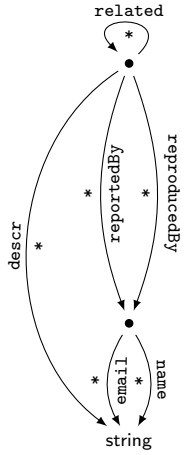


Removing a node n dominated by m

- remove n and all of its outgoing edges
- redirect its incoming edges to m

Inference of SingShEx$_0$: Reduction in detail

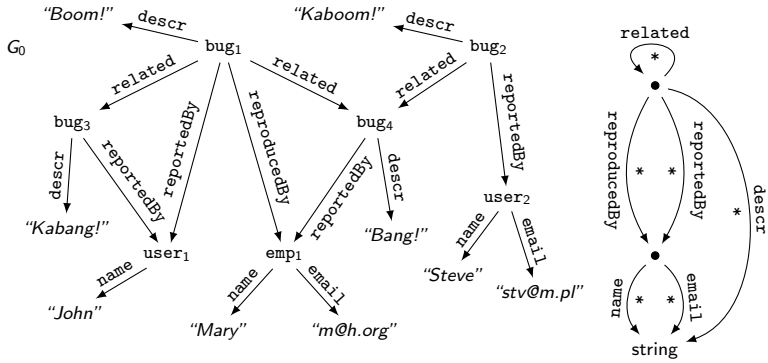
Reduce($G^\star$)



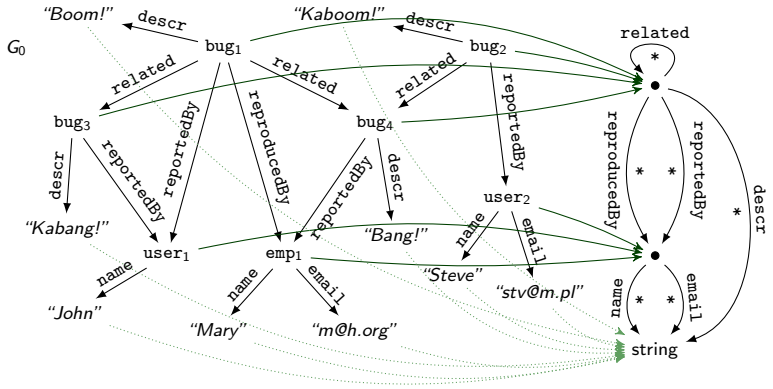
Removing a node n dominated by m

- remove n and all of its outgoing edges
- redirect its incoming edges to m

Inference of SingShEx$_0$: Specialization

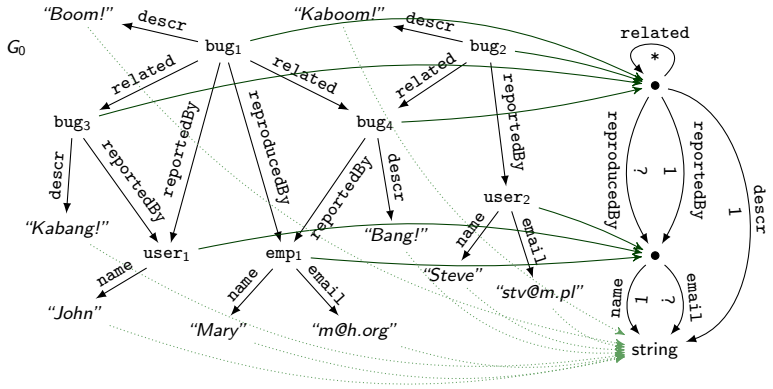


Inference of SingShEx$_0$: Specialization



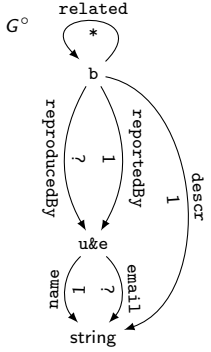
- Construct the embedding of the input graph G into the reduct of G^*

Inference of SingShEx$_0$: Specialization



- Construct the embedding of the input graph G into the reduct of G^*
- Use the embedding to replace $*$'s with fitter multiplicities

Inference of SingShEx$_0$: Specialization



- Construct the embedding of the input graph G into the reduct of G^*
- Use the embedding to replace $*$'s with fitter multiplicities

Singular Shape Expression Schemas

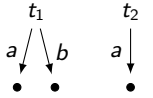
Definition (SingShEx$_0$)

A shape graph H is *singular* if

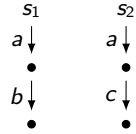
1. $H^\star$ is reduced i.e., there are no two types t_1 and t_2 in $H^\star$ that t_1 can be embedded into t_2,
2. $H^\star$ has no two edges with the same label and the same source and target nodes.

Singularity as a restriction is

- stronger than forbidding any two types t_1 and t_2 such that $t_1 \subseteq t_2$.
- weaker than forbidding any two types with comparable signatures (sets of outgoing edge labels).



Not singular



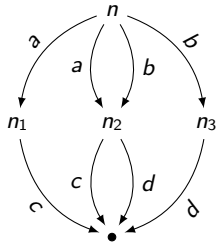
Singular

Deterministic Shape Expression Schemas

Deterministic Shape Expression Schemas

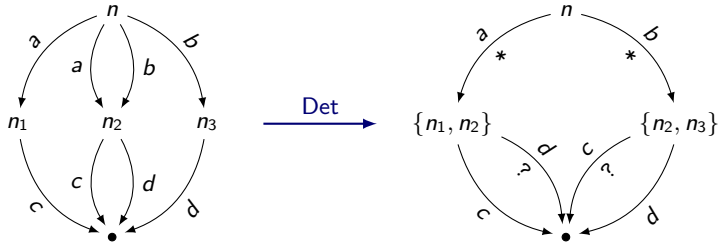
Definition ($\mathrm{DetShEx}_0$)

A shape graph H is *deterministic* if for every label a every node has at most one outgoing edges labeled with a.



Not deterministic

Determinizing Shape Graphs



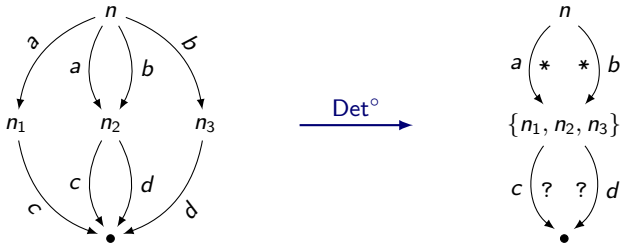
Determinization of a shape graph

- gives the fitting of the input graph
  (the $\subseteq$-minimal DetShEx$_0$ schema that validates the input graph)
- might produce exponential output

Quotient Determinization of Shape Graphs

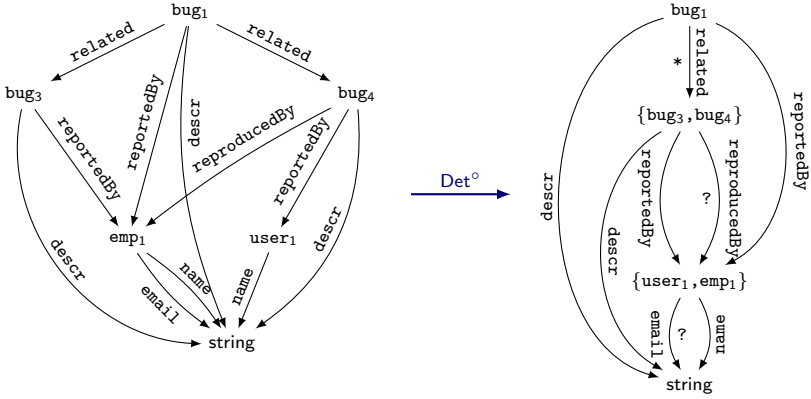
Avoid explosion by refusing to duplicate types

- if n_1 is fused with n_2 and n_2 is fused with n_3, then fuse n_1, n_2, and n_3 together.
- produces linear output



Quotient determinization is an inference algorithm for $\mathrm{DetShEx}_0^-$

Example


bug1
related
related
bug3
bug4
reportedBy
descr
reportedBy
reproducedBy
reportedBy
descr
emp1
user1
descr
name
email
name
string
Det°
bug1
*
related
reportedBy
{bug3, bug4}
reportedBy
?
reproducedBy
descr
descr
{user1, emp1}
email
?
name
string

Conclusions and Future Work

Summary

What is ShEx?

- Automata-like formalism for graphs but unlike any automata we have seen.
- Strong connections to graph bisimulation.

Complexity of Validation

	ShEx_0	ShEx	DetShEx (SORBE)
multi-type	PTIME	NP-complete	PTIME
single-type	NP-complete		

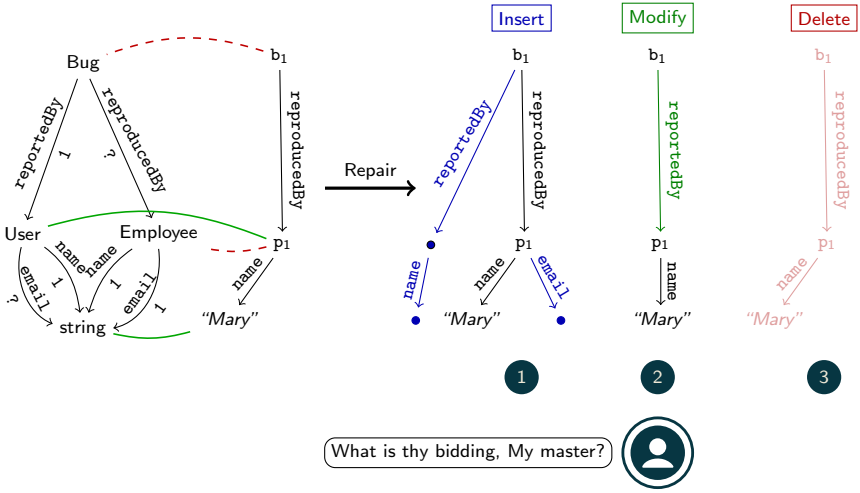
Complexity of Containment

ShEx	DetShEx(SORBE)	ShEx_0	DetShEx_0	DetShEx_0^-
coNEXP-h and co2EXP^{NP}	co2EXP	EXP-c	coNP-h	PTIME

Inference and Fitting

	ShEx_0	SingShEx_0	DetShEx_0	Typed graph
Fitting	trivial	undefined (?)	exponential	NP-hard
Inference	unfeasible	$\text{SingShEx}_0(1, *)$	DetShEx_0^-	ShEx_0 (?)

Future work: Repairing RDF



Questions

Appendix

Formal Definition of Grammatical Inference of Shape Expression Schemas

Definition

A class of shape graphs $\mathcal{C}$ is *learnable in polynomial time and data from* a class of graphs $\mathcal{G}$ iff there exists a polynomial inference algorithm A such that the following two conditions are satisfied:

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

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

When does G extend G'?

3 alternative definitions

1. G is a disjoint union of G' and some G''
2. G is obtained from G' by adding new nodes and new edges
3. as 2. but no node of G may loose a type as a result of adding outgoing edges to it.