Shape Expressions Schemas

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ABSTRACT
We present Shape Expressions (ShEx), an expressive schema language for RDF designed to provide a high-level, user friendly syntax with intuitive semantics. ShEx allows to describe the vocabulary and the structure of an RDF graph, and to constrain the allowed values for the properties of a node. It includes an algebraic grouping operator, a choice operator, cardinality constraints for the number of allowed occurrences of a property, and negation. We define the semantics of the language and illustrate it with examples. We then present a validation algorithm that, given a node in an RDF graph and a constraint defined by the ShEx schema, allows to check whether the node satisfies that constraint. The algorithm outputs a proof that contains trivially verifiable associations of nodes and the constraints that they satisfy. The structure can be used for complex post-processing tasks, such as transforming the RDF graph to other graph or tree structures, verifying more complex constraints, or debugging (w.r.t. the schema). We also show the inherent difficulty of error identification of ShEx.

1. INTRODUCTION
RDF’s distributed graph model encouraged adoption for publication and manipulation of e.g. social and biological data. Coding errors in data stores like DBpedia have largely been handled in a piecemeal fashion with no formal mechanism for detecting or describing schema violations. Extending uptake into environments like medicine, business and banking requires structural validation analogous to what is available in relational or XML schemas.

While OWL ontologies can be used for limited validation, they are generally used for formal models of reusable classes and predicates describing objects in some domain. Applications typically consume and produce graphs composed of precise compositions of such ontologies. A company’s human resources records may leverage terms from FOAF and Dublin Core, but only certain terms, and composed in specific structures. We would no more want to impose the constraints of a single human resources application suite on FOAF and Dublin Core than we would want to assert that such applications need to consume all ontologically valid permutations of FOAF and Dublin Core entities. Further, open-world constraints on OWL ontologies make it impossible to use conventional OWL tools to e.g. detect missing properties. Shape expressions define structural constraints (arc labels, cardinalities, datatypes, etc.) to provide a schema language in which it is easy to mix terms from arbitrary ontologies.

A schema language for any data format has several uses: communicating to humans and machines the “shape” of input/output data; enabling machine-verification of data on production, publication, or consumption; driving query and input interfaces; static analysis of queries. In this, ShEx provides a similar role as relational and XML schemas. Declarative switches in ShEx schemas (c.f. CLOSED and EXTRA defined below) make is useful for tightly controlled environments intolerant of extra assertions as well as linked open data media which promises a core data structure peppered with arbitrary extra triples.

ShEx validates nodes in a graph against a schema construct called a shape. In XML, validating an element against an XML Schema type or element or Relax NG production recursively tests nested elements against constituent rules. In ShEx, validating a focus node in a graph against a shape recursively tests the nodes which are the subjet or object of triples constrained in that shape.

ShEx was designed to provide a sound and coherent language without variables. The compact syntax and the JSON syntax are intended to enable trivial authoring and parsing by people and machines. The core language’s balance between expressivity and complexity is supplemented by an extension mechanism which enables more expressive semantic actions, acting like Schematron rules embedded in XML Schema or Relax NG.

Previous Work and Contributions. In [15] we presented...
a first version of shape expressions, in which we used a conjunction operator instead of grouping, and recursion was not discussed. In [19] we studied the complexity of validation of ShEx in absence of negation, and for closed shape definitions only. We showed that in general the complexity is NP-complete, identifiable tractable fragments, and proposed a validation algorithm for a restriction called deterministic single-occurrence shape expressions. In the current paper, we present an enhanced version of ShEx schemas, including the CLOSED and EXTRA modifiers, negation and well-defined recursion, value sets, and conjunction in value class constraints. We present the semantics of ShEx (Section 3) independently on regular bag expressions [19], which we believe makes it easier to understand by a larger community. We also present a full validation algorithm, as well as guidelines for its efficient implementation (Section 4). We finally show that error identification for ShEx is a hard problem, even if only the basic constructs of the language are used (Section 5). ShEx has several open-source implementations not discussed here because of space constraints, two of which can be tested online.

2. PRIMER

The following examples illustrate several features of shape expressions. Let is: be a namespace prefix for a widely-used issue tracking ontology, and foaf: and xsd: are the standard FOAF and XSD prefixes, respectively. ex: is the namespace prefix for some example instance data which we test against our example schema. ShEx uses the same conventions as Turtle [6] with relative and absolute IRIs enclosed in < > and prefixed names, as a shorthand notation for IRIs. As a convention in this primer, we will use relative IRIs as shape identifiers for our application schema.

Running Example. We give an example of a ShEx schema for data manipulated by a bug tracker. It describes five node shapes of interest. A shape describes constraints on the graph edges touching a particular node, called the focus node. The shape <TesterShape> describes the constraints for a node that represents a tester. It contains two triple constraints, that associate a property with a required value. A tester node must have one foaf:name property the object of which is a literal string value, and one is:role property the object of which is an IRI. The two triple constraints are grouped, using the comma (,) operator, indicating that the node must have triples that satisfy all parts of the grouping.

```
<TesterShape> { 
  foaf:name xsd:string, is:role IRI }
```

The shape <ProgrammerShape> requires that a node has one foaf:name that is a string, one is:experience property which value is one among is:senior and is:junior.

```
<ProgrammerShape> { 
  foaf:name xsd:string, 
  is:experience (is:senior is:junior) }
```

A user (<UserShape>) has either a foaf:givenName and a foaf:lastName, or a single foaf:name, and all these are strings. The choice between the two possibilities is expressed using the some-of operator, written as a vertical bar |. Moreover, a user has zero or more is:affectedBy properties which value satisfies <IssueShape>. The repetition constraint “zero or more” is expressed by the * symbol. A <ClientShape> is required to have only a is:clientNumber that is an integer.

```
<UserShape> { 
  (( foaf:givenName xsd:string, foaf:lastName xsd:string) 
  foaf:name xsd:string ), 
  is:affectedBy @<IssueShape> * 
} 

<ClientShape> { 
  is:clientNumber xsd:integer }
```

Finally, we describe <IssueShape>. The shape <IssueShape> specifies that the node needs to have one is:reportedBy property, whose objects satisfies both <UserShape> and <ClientShape>. Also, an issue node has to be is:reproducedBy one tester and is:reproducedBy one or more programmers. The "one or more" is written using the + sign. Additionally, an issue must have one or more inverse (i.e. incoming) is:affectedBy arc whose subject is a user; the incoming property requirement is expressed by the hat (ˆ) preceding the property. The annotations in comments (after the #) on the right of <IssueShape> will be used later on. The EXTRA modifier is explained below.

```
<IssueShape> 
  EXTRA is:reproducedBy 
  is:reportedBy @<UserShape> AND @<ClientShape>, 
  is:reproducedBy @<TesterShape>, 
  is:reproducedBy @<ProgrammerShape> + , 
  is:affectedBy @<UserShape> + } 

Here is a portion of RDF data conforming to the ShEx schema. On the right of every subject node we list the shapes satisfied by that node, and that allow to witness that ex:issue1 and ex:issue2 satisfy <IssueShape>. The edge2 annotations will be used later on.

```
ex:issue1 #<IssueShape> 
  is:reportedBy ex:fatima ; #edge1 
  is:reproducedBy ex:ren ; #edge2 
  is:reproducedBy ex:noa ; #edge3 
  is:reproducedBy ex:emin ; #edge4 
  is:dueDate "15/12/2015" xsd:date . #edge5 

ex:issue2 is:reportedBy ex:emin ; #<IssueShape> 
  is:reproducedBy ex:ren, ex:noa, ex:shristi . 
  ex:ren foaf:name "Ren Traore" ; #<TesterShape> 
  is:role is:integration ; 
  is:affectedBy ex:issue2 . 
  ex:noa foaf:name "Noa Salma" ; #<ProgrammerShape> 
  is:experience is:senior ; 
  foaf:mbox "noa@mail.com" . 
  ex:shristi foaf:name "Shristi Li" ; #<ProgrammerShape> 
  is:experience is:junior . 
  ex:fatima is:clientNumber 1 ; #<UserShape><ClientShape> 
  foaf:givenName "Fatima";
```

1Implementations: http://shex.io/#platforms/,
2Demo: http://rdfsshape.herokuapp.com/
3Demo: http://www.w3.org/2013/ShEx/FancyShExDemo
By default, the properties that are mentioned in the shape definition are allowed to appear only conforming to the corresponding constraints. For instance, a programmer cannot have a is:experience property whose value is not one among is:senior and is:junior. This default behaviour can be changed using the EXTRA modifier, that takes as parameter a list of properties. For all properties declared EXTRA, triples additional to those satisfying the triple constraints are allowed in any number, provided that their object does not satisfy the constraints being mentioned. <IssueShape> has the EXTRA is:reportedBy modifier, which allows for is:reportedBy properties whose value is neither a tester nor a programmer. Without the EXTRA modifier, the triple ex:issue1 is:reproducedBy eXem would have prevented ex:issue1 from satisfying <IssueShape>. On the other hand, even in presence of EXTRA, an issue shape can still be is:reproducedBy only one tester.

Regarding the properties not mentioned in the shape definition, they are by default in any number with unconstrained values. For instance, a programmer can have a foaf:mbox property, and an issue can have a is:dueDate. This default behaviour can be tuned too: the CLOSED modifier forbids all properties that are not mentioned in the shape definition, and the OPEN modifier forbids all inverse properties not mentioned. The modifiers CLOSED and EXTRA can be combined, in order to forbid all non mentioned properties, except for those that are arguments of EXTRA.

ShEx schemas also include a negation operator !. For instance, one could define an issue having low impact as an issue that is possibly reproduced and reported several times, but not by a client.

\[
\text{<LowImpactIssueShape> \{ 
  \text{is:reportedBy} \text{!}@\text{<ClientShape>}, 
  \text{is:reproducedBy} \text{!}@\text{<ClientShape>}
\} 
\]

The Running Example can be tested online.

**Repeated Properties.** Much of the design of ShEx arises from meeting use cases with multiple triple constraints on the same property (or Repeated Properties) as seen above in <IssueShape> which requires is:reproducedBy arcs for at least one tester and at least one programmer. These are quite common in clinical informatics where generic properties relate observations in specific ways, but in fact emerge any time a schema or convention re-purposes generic predicates. Because RDF is a graph, the same node may be involved in the validation of multiple triples where that node matches multiple shapes. For instance, consider a small modification of the Running Example, by adding the triple ex:shristi is:role is:integration.

Then ex:shristi satisfies both <ProgrammerShape> and <TesterShape>. Validating ex:issue2 as a <IssueShape> requires ex:shristi to be seen as a programmer, as ex:ren satisfies only <TesterShape>. A less nuanced interpretation would treat all repeated properties in a shape as a conjunction of constraints, in which case ex:issue2 would not match <IssueShape> because ex:ren would have to match both <ProgrammerShape> and <TesterShape>.

**Extension Mechanism and JSON Syntax.** ShEx schemas have two additional features that we do not present here because of space constraints. The extension mechanism presented also in [15], allows to decorate schemas with executable code, called semantic actions, which are useful for more expressive validation. For instance, a semantic action might be used to check value ranges or invoke a service to test membership in an external value set:

\[
\text{<ClientShape> \{}
  \text{is:clientNumber} \text{xsd:integer,}
  \%\text{ex:memberOf}\{\text{ex:OurClients}\}
\text{\} }
\]

Semantic actions can also produce output to e.g. construct XML fitting some XML schema.

The examples in this section are all presented with what is called the compact syntax or ShExC, that is intended to be processed by humans. ShEx schemas are easier to programmatically use and manipulate using the JSON syntax, and round-trip translators.

### 3. Syntax and Semantics of ShEx

#### 3.1 Abstraction of RDF Graphs

Shape expression schemas allow to constraint both the incoming and outgoing edges of a node. In order to handle incoming and outgoing edges uniformly, we consider an abstraction of RDF graphs. Let Prop be a set of properties, that in practice correspond to the set of IRI, and let ~Prop be the set of inverse properties. An inverse property is simply a property decorated with the hat `^`, that is, if prop is a property, then `^prop` is an inverse property.

A graph is defined by a set of nodes Nodes, a set of edges Edges, and a value function val. The nodes of the graph are abstract entities. The value function val associates, with every node in Nodes, either an IRI, or a literal value, or a special value `b` that stands for a blank node. Finally, every edge in Edges is a triple of the form `(node, q, node')`, where node and node' are two nodes, and q is a property or an inverse property. The nodes node and node' are called the source and the target nodes of the edge, respectively.

Given a set of triples defining an RDF graph, the above abstraction is obtained by:

- For all IRI I that appears in the subject or object position in some triple, there is nodeI in Nodes such that val(nodeI) = I.
• For all blank node $B$ that appears in some triple, there is a node$_B$ in Nodes such that val(node$_B$) = _b.

• For all triple (subj, prop, obj), the set Edges contains the forward edge (node$_{subj}$, prop, node$_{obj}$) and the inverse edge (node$_{obj}$, prop, node$_{subj}$).

Given a node in a graph, its neighbourhood is the set of its adjacent edges, that is, the edges of the form (node, prop, node') and (node', prop, node) that belong to Edges. We denote this set by neigh(node). For instance, on the Running Example, the neighbourhood of the node nodeex:issue1 is composed of the edges (that correspond to the triples) edge1, . . . , edgen and the inverse of edgen. A set of neighbourhood edges is a subset of the neighbourhood of some node.

3.2 Syntax of ShEx Schemas

In the abstract syntax presented here, we omit the curly braces that enclose shape definitions, and the @ sign preceding referenced shape names. A shape expression schema (ShEx schema) defines a set of shape labels and their associated shape definitions.

ShapeExprSchema ::= (ShapeLabel ShapeDefinition)*

ShapeDefinition ::= 'CLOSED'? '¬CLOSED'?
(ExtraPropSet)? ShapeExpr

ExtraPropSet ::= a set of properties or inverse properties

A shape definition is composed of a shape expression (ShapeExpr), possibly preceded by the optional modifiers CLOSED (forward closed), ¬CLOSED (inverse closed) or EXTRA, the latter taking as parameter a set of properties or inverse properties.

A shape expression specifies the actual constraints on the neighbourhood, and is defined by the following syntax rule:

ShapeExpr ::= EmptyShape | TripleConstraint | SomeOfShape | GroupShape | RepetitionShape

The empty shape (EmptyShape) imposes no constraints. An empty (forward) CLOSED shape can only be satisfied by a node without outgoing edges, while an empty shape that is not (forward) CLOSED can have any outgoing edges.

The basic component of a shape expression is a triple constraint.

TripleConstraint ::= (Property | InvProperty) ValueClass
Property ::= an IRI
InvProperty ::= →Property

A triple constraint is either a forward constraint of the form prop K, or an inverse constraint of the form 'prop K. A triple constraint is satisfied by a single edge adjacent to the focus node which node opposite to the focus node satisfies the constraint defined by K, and which label is the property of the triple constraint. Examples of triple constraints are foaf:name xsd:string and is:reportedBy @<UserShape> AND @<ClientShape>. If the focus node is node, then an edge (node, foaf:name, node') satisfies the triple constraint foaf:name xsd:string if val(node') is a string. The form of the ValueClass constraint K is described below.

A some-of shape expression defines a disjunctive constraint.

SomeOfShape ::= ShapeExpr ("|" ShapeExpr)^

It is composed by one or more sub-expressions, separated by the | sign. A some-of expression is satisfied by a set of neighbourhood edges if at least one of its sub-expressions is satisfied. An example of a some-of shape is foaf:givenName xsd:string | foaf:firstName xsd:string.

A group shape expression is composed by one or more sub-expressions, separated by the comma sign.

GroupShape ::= ShapeExpr ("," ShapeExpr)*

It is satisfied by a set of neighbourhood edges if the set can be split into as many disjoint subsets, and each of these components satisfies the corresponding sub-expression. An example of a group shape is (foaf:givenName xsd:string | foaf:firstName xsd:string), foaf:mbox xsd:string.

Finally, a repetition shape expression is composed by an inner sub-expression, and an allowed number of repetitions specified by a possibly unbounded interval of natural values.

RepetitionShape ::= ShapeExpr Cardinality
Cardinality ::= [ MinCardinality ';'; MaxCardinality ]
MinCardinality ::= a natural number
MaxCardinality ::= a natural number | 'unbound'

Its satisfiability is similar to that of a group expression. A set of neighbourhood edges satisfies a group expression if it can be split into as many disjoint subsets, each of which satisfies the sub-expression, where m must belong to the interval of allowed repetitions. An example of a repetition shape is is:reproducedBy @<ProgrammerShape>, where + is a short for the interval [1, unbound].

Hera are the constraints defined by ValueClass:

ValueClass ::= AtomicConstr ("AND" AtomicConstr)*
AtomicConstr ::= ValueSet | ShapeConstr
ValueSet ::= set whose elements are literals, IRIs, or _b
ShapeConstr ::= ShapeLabel | "!"ShapeLabel
ShapeLabel ::= an identifier

It is a conjunction of sets of values (ValueSet), and of shape constraints (ShapeConstr). A ValueSet can contain IRIs, literal values, or the special constant _b for a blank node. In practice, it can be given by listing the values (such as (is:senior is:junior)), by an XS string type (such as xsd:string, xsd:integer), by a node kind specification (for example IRI, blank, literal, non-literal), by a regular expression defining the allowed IRIs, etc. A neighbour node of the focus node satisfies a ValueSet constraint if its value belongs to the corresponding set. A shape constraint ShapeConstr is either a shape label, or a negated shape label, that is a shape label preceded by the bang (!) symbol. A neighbour node of the focus node satisfies a non negated ShapeLabel if its neighbourhood satisfies the shape definition that corresponds to that shape label. A negated ShapeLabel is satisfied by a node if its neighbourhood does not satisfy the corresponding shape definition.
3.3 Well-defined Schemas

We assume a fixed ShEx schema Sch whose set of labels is Shapes. For a shape label S, we denote by definition(S) its shape definition in Sch, and by expr(S) the shape expression within the definition of S.

The dependency graph of the schema Sch describes how shape labels refer to each other in shape definitions. More formally, the dependency graph of Sch is an oriented graph whose nodes are the elements of Shapes, and that has an edge from S to T if the shape label T appears in some triple constraint in expr(S).

Let S and T be shape labels. We say that $T$ appears negated in definition(S) if either $T$ appears in definition(S), or there is some triple constraint $q X_1$ AND ... AND $X_k$ in expr(S) such that $q$ is an extra property in definition(S), and $T$ is a shape label among $X_1, \ldots, X_k$. For instance, in the Running Example, the shape labels <TesterShape> and <ProgrammerShape> appear negated in the definition of <IssueShape> because is:reportedBy is an extra property. We denote by negated-shapes(S) the set of shape labels that appear negated in definition(S), and negated-shapes(Sch) is the union of negated-shapes(S) for all S in Shapes.

The following syntactic restriction is imposed in order to guarantee well-defined semantics for ShEx schemas in presence of recursion and negation. It requires that shape labels that appear negated do not lead to cyclic dependencies between shapes. From now on, we assume that all schemas are well-defined.

Definition 1 (Well-defined schema) A shape expression schema Sch is well-defined if for every shape labels S, T, if T is in negated-shapes(S), then the sub-graph accessible from T in the dependency graph of Sch is a direct acyclic graph.

3.4 Declarative Semantics of ShEx

Locally Satisfying a Shape Definition. For every shape definition, we need to refer to the occurrences of its triple constraints. Therefore, we are going to use $C_1, \ldots, C_k$ as unique names for the triple constraints that appear in a shape definition. The shape definition to which the $C_i$ belong will be clear from the context. Note that if the same triple constraint appears twice (i.e. same property and same value class), the two occurrences are distinguished and correspond to different $C_i$’s. To say it differently, any of the $C_i$ corresponds to a $\text{TripleConstraint}$-position in the abstract syntax tree of a shape definition.

For every shape definition we identify a set of triple consumers, that correspond either to some triple constraint, or to an extra property, or to the unconstrained properties of open (i.e. not closed) shape definitions. Intuitively, a node locally satisfies a shape definition if all edge from $\text{neigh}(node)$ can be consumed by one of the triple consumers of that shape definition, in a way that satisfies its shape expression.

Formally, let ShDef be a shape definition (fixed in the sequel), and let $C_1, \ldots, C_k$ be the set of its triple constraints. The set of triple consumers of ShDef consists of:

- $\text{TCons}_{\text{open}}$ for all extra property $q$ in ShDef;
- $\text{TCons}_{\text{extra}}$ for all extra property $q$ in ShDef;
- $\text{TCons}_{\text{open}}$ which is a special constant.

We say that an edge $\text{edge} = (\text{node}, q, node')$ matches a triple consumer $\text{TCons}$ if either $\text{TCons} = \text{TCons}_{\text{extra}}$, or $\text{TCons} = \text{TCons}_{\text{open}}$ with $C_q = q X_i$ AND ... AND $X_k$ and for all $1 \leq j \leq k$ such that $X_j$ is a value set, it holds that $\text{val}(node') \in X_j$.

Definition 2 (Local witness) Let ShDef be a shape definition, Consumers be the its set of triple consumers, and let node be a node. Let witness : $\text{neigh}(node) \rightarrow \text{Consumers}$ be a total mapping that maps a triple consumer with every edge in $\text{neigh}(node)$. We say that the mapping witness is a local witness for the fact that $\text{neigh}(node)$ satisfies ShDef, written witness, $\text{neigh}(node) \vdash \text{ShDef}$, iff:

- For all edge $\text{edge} = (\text{node}, q, node')$ in $\text{neigh}(node)$:
  - edge matches witness(edge) whenever witness(edge) is of the form $\text{TCons}_{\text{extra}}$ or $\text{TCons}_{\text{open}}$;
  - if witness(edge) = $\text{TCons}_{\text{extra}}$, then there is no $\text{TCons}_{\text{open}}$ in Consumers s.t. and all the conjuncts in $C_q$, are value sets and edge matches $\text{TCons}_{\text{extra}}$;
  - if witness(edge) = $\text{TCons}_{\text{open}}$, then Consumers does not contain any triple consumer of the form $\text{TCons}_{\text{extra}}$ or $\text{TCons}_{\text{open}}$ with $C_q$ of the form $q K$ (i.e. having the same property $q$).

- If ShDef is forward closed (respectively, inverse closed), then there is no forward edge (respectively, inverse edge) that is mapped with $\text{TCons}_{\text{open}}$ by witness.

- Let $\text{Neigh}_{\text{expr}}$ be the set of edges $\text{edge}$ from $\text{neigh}(node)$ such that witness(edge) = $\text{TCons}_{\text{open}}$ for some triple constraint $C_q$ in ShDef, then it holds that witness, $\text{Neigh}_{\text{expr}} \vdash \text{expr(ShDef)}$.

For a set of neighbourhood edges Neigh, a shape expression Expr, and a mapping witness : Neigh $\rightarrow$ Consumers, we say that witness is a local witness for the fact that Neigh satisfies Expr, written witness, Neigh $\vdash$ Expr, iff:

- $\text{Expr}$ is the empty shape, and Neigh = $\emptyset$;
- $\text{Expr} = C_i$ is a triple constraint, Neigh = $\{\text{edge}\}$ is a singleton set, and witness(edge) = $C_i$;
- $\text{Expr} = \text{Expr}_1 \mid \ldots \mid \text{Expr}_k$ is a some-of shape, and witness, Neigh $\vdash \text{Expr}_i$ for some $1 \leq i \leq k$.
- $\text{Expr} = \text{Expr}_1, \ldots, \text{Expr}_k$ is a group shape, and for all $1 \leq i \leq k$, denote by Neigh$_i$ the subset of Neigh that contains edge iff witness(edge) = $TCons_{C_i}$ for some triple constraint $C_j$ in $\text{Expr}_i$. Then it holds that Neigh = Neigh$_1 \cup \ldots \cup$ Neigh$_k$, and witness, Neigh$_i \vdash \text{Expr}_i$ for all $1 \leq i \leq k$.
- $\text{Expr}[\text{min} ; \text{max}]$ is a repetition shape, and there exists m that belongs to the interval $[\text{min} ; \text{max}]$ such that one can partition Neigh in m disjoint sets Neigh$_1, \ldots, \text{Neigh}_m$, whose union is Neigh, and such that witness, Neigh$_i \vdash \text{Expr}$ for all $1 \leq i \leq m$. □
Example 3.1 With the schema and data from the Running Example, and with $T_{Cons}$ as short for $T_{Cons_{\text{reproducedByExtra}}}$, we have that $edge_1$ matches $T_{Cons_{\text{c1}}}$, $edge_2$ matches $T_{Cons_{\text{open}}}$, (the inverse of) $edge_3$ matches $T_{Cons_{\text{c4}}}$, and $edge_4$ matches $T_{Cons_{0}}$, $T_{Cons_{\text{c2}}}$, $T_{Cons_{\text{c3}}}$, for $j = 2, 3, 4$. The mapping witness defined hereafter is a local witness for the fact that $T_{Cons}$ Shapes (the inverse of) $Sch_{immediate}$ neighbourhood of a node. Thus, the validity of a shape labels of the form $!_\text{GlobalTypingWitness}$. The shape labels that appear in $Sch$ node precisely the couples $(\text{nodes}, \text{nodes})$ such that $(\text{nodes}), \text{nodes})$ matches $T_{Cons_{\text{c1}}}$, $T_{Cons_{\text{open}}}, T_{Cons_{\text{c4}}}$, $T_{Cons_{0}}$, $T_{Cons_{\text{c2}}}$, $T_{Cons_{\text{c3}}}$, for $j = 2, 3, 4$.

Global Typing Witness. The shape labels that appear in triple constraints allow to propagate constraints beyond the immediate neighbourhood of a node. Thus, the validity of a graph with respect to a ShEx schema is a global property on the graph, and is captured by the notion of a global typing witness to be defined shortly.

As previously, we consider a ShEx schema $Sch$ whose set of shape labels is $Shapes$. Let $NegatedShapes$ be the set of shape labels of the form $!_\text{S}$ where $S$ is in negated-shapes$(Sch)$. That is, $NegatedShapes$ contains all the shapes that appear negated in $Sch$, decorated by a leading $\neg$ sign.

A typing of a graph $G$ by $Sch$ is a set typing $\subseteq$ $Nodes \times (Shapes \cup NegatedShapes)$ of couples of the form $(\text{node}, S)$ or $(\text{node}, !_\text{S})$, and such that there is no node and no shape label $S$ for which both $(\text{node}, S)$ and $(\text{node}, !_\text{S})$ belong to typing. Let witness be a local witness, then the propagation of witness is the typing propagation witness that contains precisely the couples $(\text{node}, X)$ for all edge $(\text{node}, q, \text{nodes})$ in the domain of witness such that witness$(\text{node}, q, \text{nodes})$ = $T_{Cons_{\text{c1}}}$, corresponds to a triple constraint $C_i$, and $X$ is a shape label or negated shape label that appears as a conjunct in $C_i$.

Definition 3 (Global typing witness) A global typing witness for a graph $G$ by a schema $Sch$ is a couple typing, lw, where typing is a typing of $G$ by $Sch$, and lw is a total map from typing $\cap (Nodes \times Shapes)$ to local witnesses, s.t. for all $(\text{node}, S)$ in typing, it holds that lw$(\text{node}, S)$ is a local witness for the fact that $\text{node}$ satisfies definition$(S)$. Additionally:

$$
gtw\text{-extra-shape-constr} \text{ or } X_j \text{ is a shape constraint, and there exists a global typing witness typing}', lw' \text{ such that } (\text{node}', Y_j) \in \text{typing}', \text{where } Y_j = 1_X, \text{ if } X_j \text{ is a shape label, and } Y_j = T \text{ if } X_j = !T \text{ is a negated shape label.} \Box
$$

Example 3.2 With the shape and data from the Running Example, and with witness from Example 3.1 there is no global typing witness that includes propagation witness, because (exemin, $<\text{ProgrammerShape}>$) is in propagation witness and exemin does not satisfy $<\text{ProgrammerShape}>$. Let typing be the typing that with every subject node of the Running Example associates the shape labels listed in the comment on the right of that node in the example data, e.g. typing contains $(\text{excren}, <\text{TesterShape}>)$, $(\text{exfatima}, <\text{UserShape}>)$, $(\text{exfatima}, <\text{ClientShape}>)$, etc. Then typing corresponds to a global typing witness, with lw$(\text{node}_{\text{excren}}, <\text{IssueShape}>)$ = witness’, with witness’ identical to witness except for edge$4 \mapsto T_{Cons_{0}}. \Box$

The definition of a global typing witness is recursive: in the $gtw\text{-neg}$ we require to ensure that some typing$, lw$ is not a global typing witness in order to ensure that typing, lw is a global typing witness. It what follows, we give some fundamental properties of global typing witnesses that allow to show that the definition is well-founded.

Theorem 3.3 For all graph $G$ and all shape expression schema $Sch$, there exists a global typing witness typing$^\text{cert}$, lw$^\text{cert}$, $Sch$, lw$^\text{cert}$ such that for all node $\text{node}$ in $G$ and all shape label $S$ in negated-shapes$(Sch)$, either $(\text{node}, S)$ or $(\text{node}, !_\text{S})$ belongs to typing$^\text{cert}$.

Proof. (Sketch.) We sketch the proof using an example, and show how typing$^\text{cert}$, lw$^\text{cert}$ can be effectively computed, starting with an empty typing. The proof is based on the well-founded criterion of schemas. Suppose that negated-shapes$(Sch)$ = $\{S_1, S_2, S_3, S_4\}$ and the dependency among them is $S_1 \rightarrow S_2$, $S_1 \rightarrow S_3$, $S_2 \rightarrow S_4$, $S_3 \rightarrow S_1$ (where $S_1 \rightarrow S_2$ means that $S_2$ appears in the definition of $S_1$). We start by typing with $S_4$, as follows. For all node, if there exists a local witness for the fact that node satisfies $S_4$, then we add $(\text{node}, S_4)$ to typing$^\text{cert}$, and we set lw$^\text{cert}$(node, $S_4$) = witness’. Otherwise, we add $(\text{node}, !_S_4)$ to typing$^\text{cert}$. After this first step, typing$^\text{cert}$, lw$^\text{cert}$ is a global typing witness. Indeed, it satisfies $gtw\text{-sat}$ by definition. For $gtw\text{-neg}$, suppose by contradiction that $(\text{node}, S_4)$ in typing$^\text{cert}$ and there is a global typing witness typing’, lw’ s.t. $(\text{node}, S_4) \in \text{typing}', \text{then lw'}(\text{node}, S_4) \text{ is a local witness for the fact that node satisfies } S_4; \text{ this is a contradiction.}$ For $gtw\text{-extra}$, the proof goes again by contradiction: if lw$^\text{extra}$$(\text{node}, S_4), (\text{node}, q, \text{nodes}) = T_{Cons_{\text{extra}}}$ and there is $T_{Cons_{\text{extra}}}$ consumer in the definition of $S_4$ such that $\text{node}$ is in val$(X_j)$ for all $X_j$ conjunct in $C_i$, then lw$^\text{extra}$(node, $S_4$) does not satisfy the definition of local witness: contradiction.

We next associate the shapes $S_2$ and $S_3$ to all nodes. We can do it in any order, because they both only depend on $S_4$. We illustrate taking $S_2$. Let typing$^\text{prev}$, lw$^\text{prev}$ be typing$^\text{cert}$, lw$^\text{cert}$ as obtained during the previous step (i.e., typing$^\text{prev}$ uses only $S_2$ and $!\text{S}$ as shapes). For all node, if there exists a local witness for the fact that node satisfies $S_2$
and s.t. \( \text{propagation}_{\text{witness}} \subseteq \text{typing}^{\text{prev}} \), we add \((\text{node}, S_2)\) to \(\text{typing}^{\text{cert}}_{G, \text{Sch}}\); otherwise we add \((\text{node}, S_3)\) to \(\text{typing}^{\text{neg}}_{G, \text{Sch}}\). Using similar arguments as for the previous step, and that \(\text{typing}^{\text{prev}} \subseteq \text{typing}^{\text{neg}}\) is a global typing witness, we show that the new \(\text{typing}^{\text{cert}}_{G, \text{Sch}}, \text{lw}^{\text{cert}}_{G, \text{Sch}}\) is a global typing witness too.

This process is repeated until all negated shape labels have been processed, and following the order inducing by the (acyclic) dependency graph. For instance, \(S_1\) can be added only after \(S_2\) and \(S_3\) are both added.

The following Corollary 3.4 establishes that all global typing witness agrees with \(\text{typing}^{\text{cert}}_{G, \text{Sch}}, \text{lw}^{\text{cert}}_{G, \text{Sch}}\) on the shape labels that appear negated in \(\text{Sch}\). It follows from the proof of Theorems 3.3 and from Definition 3. This allows us to give an equivalent, non recursive definition for a global typing witness in Lemma 3.5

**Corollary 3.4** If \(\text{typing}, \text{lw}\) is a global typing witness for the graph \(G\) by the schema \(\text{Sch}\), then for all \(S \in \text{negated-shapes}(\text{Sch})\), and for all node \(\text{node}\) in \(G\), if \((\text{node}, S) \in \text{typing}\), then \((\text{node}, S) \in \text{typing}^{\text{cert}}_{G, \text{Sch}}\), and if \((\text{node}, S) \in \text{typing}\), then \((\text{node}, S) \in \text{typing}^{\text{neg}}_{G, \text{Sch}}\).

**Lemma 3.5** In Definition 3 the \(\text{gtw-neg}'\) and \(\text{gtw-extra-shape-constr}'\) conditions can be replaced by the following weaker conditions \(\text{gtw-neg}^\prime\) and \(\text{gtw-extra-shape-constr}'\) respectively, while leaving the underlying notion of global typing witness unchanged:

\[
\text{gtw-neg}'(\text{node}, !S) \in \text{typing} \quad \text{only if} \quad (\text{node}, !S) \in \text{typing}^{\text{cert}}_{G, \text{Sch}}.
\]

\[
\text{gtw-extra-shape-constr}' \quad \text{or} \quad X_j \text{ is a shape constraint, and} \quad (\text{node}', Y_j) \in \text{typing}^{\text{cert}}_{G, \text{Sch}}, \text{ where } Y_j = !X_j \text{ if } X_j \text{ is a shape label, and } Y_j = T \text{ if } X_j = !T \text{ is a negated shape label.}
\]

### 4. Validation Algorithm

The fundamental question in validation is “does \(X\) satisfy \(Y\)?”, e.g. “does \(\text{ex:issue}\) satisfy \(<\text{IssueShape}>\)?”. Following is a validation algorithm which, given an initial typing \(\text{typing}_i\), that contains typing requirements such as \(\text{ex:issue1}, \text{IssueShape}\), constructs a global typing witness \(\text{typing}_i\) that includes \(\text{typing}_i\) if one exists, and raises a validation error otherwise. Throughout the section we consider a fixed graph \(G\) with nodes \(\text{Nodes}\), edges \(\text{Edges}\) and a value function \(\text{val}\), a fixed shape expression schema \(\text{Sch}\) over a set of shape labels \(\text{Shapes}\), and a fixed (partial) initial typing \(\text{typing}_i\) of \(G\) by \(\text{Sch}\). We start by presenting a high-level version of the algorithm, and then discuss some implementation and optimization aspects.

**4.1 Data Structures**

The flooding algorithm produces a global typing witness. It proceeds by making \(\text{typing} \) hypotheses, that are associations of a node and a shape label. The algorithm tries to witness that each such hypothesis is satisfied, or otherwise removes it, until a global typing witness is obtained. The satisfaction of a typing hypothesis might require other typing hypotheses to be satisfied. During its computation, the algorithm maintains a structure called \(\text{typing} \) witness under construction denoted \(\text{TUC}\), which contains the current hypotheses, together with additional data useful for the computation.

More precisely \(\text{TUC} = (\text{typing}^{\text{hyp}}, \text{lw}^{\text{hyp}}, \text{requires}, \text{toCheck})\), where \(\text{typing}^{\text{hyp}}, \text{lw}^{\text{hyp}}\) is the global typing witness under construction, \(\text{requires} \subseteq \text{typing}^{\text{hyp}} \times \text{typing}^{\text{hyp}}\) is a binary relation on hypotheses, and \(\text{toCheck}\) is a subset of \(\text{typing}^{\text{hyp}} \cap (\text{Nodes} \times \text{Shapes})\) of not yet verified hypotheses. We suppose that \(\text{typing}^{\text{cert}}_{G, \text{Sch}}, \text{lw}^{\text{cert}}_{G, \text{Sch}}\) is given, denoted \(\text{typing}^{\text{cert}}, \text{lw}^{\text{cert}}\) for short.

Finally, the algorithm uses a global map \(\text{UnchLW}\) that, with every node \(\text{node}\) and shape label \(\text{S}\), associates the set of local witnesses that can potentially be used for proving that \(\text{node}\) satisfies \(\text{S}\). A local witness \(\text{witness}\) is removed from \(\text{UnchLW}(\text{node}, \text{S})\) when we know that it cannot be used in any global typing witness, that is, when there does not exist a global typing witness \(\text{typing}, \text{lw}\) s.t. \((\text{node}, \text{S})\) belongs to \(\text{typing}\) and \(\text{propagation}_{\text{witness}}\) is included in \(\text{typing}\).

**4.2 The Flooding Algorithm**

The flooding algorithm is presented in Algorithm 1. It starts by checking whether the initial typing \(\text{typing}_i\) is compatible with the certain types \(\text{typing}^{\text{cert}}\), and if not, it signals a validation error. Otherwise, the typing under construction is initialized so that it contains \(\text{typing}_i\) as initial hypotheses, all the initial hypotheses involving a non-negated shape label are added to \(\text{toCheck}\), whereas the \(\text{lw}^{\text{hyp}}\) and \(\text{requires}\) components are empty (lines 3 to 9). The function \(\text{checkCompatible}\) takes as parameters two typings and returns false iff there are a node \(\text{node}'\) and a shape label \(\text{T}\) s.t. one of the typings contains \((\text{node}', \text{T})\) and the other contains \((\text{node}', !\text{T})\).

The main loop on line 10 iterates on all hypotheses in \(\text{toCheck}\), until all have been processed. For all hypothesis \((\text{node}, \text{S})\) in \(\text{toCheck}\), we distinguish three possible cases, that are the conditions on lines 10 to 12. On line 10 the hypothesis \((\text{node}, \text{S})\) to be checked is known to be verified because \(\text{S}\) is a certain type for \(\text{node}\). Line 10 corresponds to the case where the hypothesis \((\text{node}, \text{S})\) is recognized as non provable because the set \(\text{UnchLW}(\text{node}, \text{S})\) of unchecked hypotheses is empty. We need to backtrack, as explained later on. Finally, line 12 corresponds to the case when there exists a local witness \(\text{witness}\) that has not been used yet for verifying whether \(\text{node}\) satisfies \(\text{S}\). Then we first use the Boolean functions \(\text{checkGtwExtra}(\text{see below})\) to make sure that \(\text{witness}\) does not violate the \(\text{gtw-extra}\) condition, and \(\text{checkCompatible}\) to make sure that propagating the witness won’t contradict the certain typing. If the check passes, then we set \(\text{lw}^{\text{hyp}}(\text{node}, \text{S})\) to \(\text{witness}\) (line 13), meaning that we are going to look for a valid typing compatible with \(\text{witness}\), then we propagate the further requirements imposed by \(\text{witness}\) to the neighbours of \(\text{node}(\text{lines 16 to 23})\).

Otherwise (line 23), \(\text{witness}\) is removed from \(\text{UnchLW}\), and \((\text{node}, \text{S})\) is added back to \(\text{toCheck}\) for further checking. The functions \(\text{checkGtwExtra}\) takes as input a schema \(\text{Sch}\), a shape label \(\text{S}\), a local witness \(\text{witness}\), and a certain typing \(\text{typing}^{\text{cert}}\), and returns false iff there is an edge \(\text{edge} = (\text{node}, q, \text{node}')\) in the domain of witness s.t. \(\text{witness} (\text{edge}) = \text{TCons}_{\text{q}, \text{extra}}\) is an extra consumer, and there exists a triple consumer \(\text{TCons}_{\text{C}}, \text{in the definition of S (in Sch)}\) such that \((\text{node}', \text{X}) \in \text{typing}^{\text{cert}}\), for all shape constraint \(\text{X}\) that is a conjunct in \(\text{C}\).

When all the hypotheses have been processed (line 26), \(\text{typing}^{\text{hyp}}, \text{lw}^{\text{hyp}}\) is (almost) a global typing witness. However, it might not contain \(\text{typing}_i\), because some of the initially required hypotheses have been disproved (removed during backtracking-
Algorithm 1: FloodingValidation
Input: Sch a shape expression schema over Shapes,
       G = (Nodes, Edges, val) a graph,
       typing a pre-typing of G by Sch,
       UnchLW a map from Nodes × Shapes to sets of local witnesses
       typing^{cert}, lw^{cert} a global typing witness
Output: typing, lw a global typing witness
1: if not checkCompatible(typing, typing^{cert}) then
   return VALIDATION_ERROR
2: let TUC := (typing^{hyp}, lw^{hyp}, requires, toCheck), where
3:     typing^{hyp} = typing_{0}, lw^{hyp} = \emptyset, requires = \emptyset,
4:     and toCheck = typing_{0} \cap (Nodes \times Shapes)
5: while toCheck \neq \emptyset do
6:     (node, S) := remove from toCheck
7:     if (node, S) \in typing^{cert} then
8:         continue
9:     else if UnchLW(node, S) = \emptyset then
10:        Backtracking(node, S, TUC)
11:     else
12:        witness := get first from UnchLW(node, S)
13:        if checkGtwExtra(Sch, S, witness, typing^{cert}) and
14:           checkCompatible(propagation_{witness}, typing^{cert}) then
15:            lw^{hyp}(node, S) = witness
16:            foreach (node', X) in propagation_{witness} do
17:                if (node', X) \notin typing^{hyp} then
18:                    add (node', X) to typing^{hyp}
19:                    if X \in Shapes then
20:                        add (node', X) to toCheck
21:                    else
22:                        remove witness from UnchLW(node, S)
23:                        add (node, S) to toCheck
24:            if typing_{0} \subseteq typing^{hyp} then
25:                foreach (node, S) \in typing^{hyp} \land typing^{cert} do
26:                    copyProof(node, S, typing^{cert}, lw^{cert}, typing^{hyp}, lw^{hyp})
27:            return typing = typing^{hyp}, lw = lw^{hyp}
28:        else
29:            return VALIDATION_ERROR

Algorithm 2: Backtracking
Input: (node, S) a hypothesis,
       TUC = (typing^{hyp}, lw^{hyp}, requires, toCheck)
       a global typing witness under construction
1: foreach (node', S') \in toRemove(node, S, requires) do
2:     remove (node', S') from typing^{hyp}, lw^{hyp}, and toCheck
3:     for all (node', S') s.t. requires((node', S'), (node, S)),
       (node', S') is in toRemove(node, S, requires):
6:       if (node', S') is such that for all (node'', S'') we have
7:           that requires((node'', S''), (node', S')) implies (node', S'') \in
8:           toRemove(node, S, requires), then (node', S') is also in
9:           toRemove(node, S, requires).

Additionally, in the loop on line ??, backtracking invalidates the local witnesses for the hypotheses (node', S') that required (node, S), and adds them back for checking.

Computing the Sets of Unchecked Local Witnesses.
Let node be a node, S be a shape label which definition contains the triple constraints C_1, ..., C_k and has corresponding set Consumers of triple consumers. We compute the set UnchLW(node, S) by considering a set of candidate mappings from neigh(node) to Consumers, and keeping those candidates that are actual local witnesses for the fact that node satisfies the definition of S. A mapping is a candidate if it associates with every edge a triple consumer that this edge matches. More formally, for all edge = (node, q, node'), let matchingTC(edge) = \{TC_{cons_{\text{span}}} \} if q does not appear in any of C_i, neither as an extra property in S, and matchingTC(edge) = \{TC_{cons_{\text{extra}}} \} \cup \{TC_{\mid \text{edge matches } TC_{\mid \text{edge}}} \} otherwise. Then a candidate mapping is obtained by choosing one triple consumer among matchingTC(edge) for all edge in neigh(node).
For instance, continuing Example [3.3], a candidate map from neigh(node_{\text{issue1}}) to the triple consumers of <IssueShape> will always associate TC_{cons_{\text{span}}} with edge_{\text{s}}, and will associate one among TC_{cons_{\text{a}}}, TC_{cons_{\text{c}}}, and TC_{cons_{\text{c}}} with edge_{\text{g}}.
We denote CandidateULW(node, S) the set of candidate mappings, and it is obtained as the Cartesian product of the sets matchingTC(edge), for all edge in neigh(node).

Once the set CandidateULW(node, S) of candidate mappings is constructed, we have to determine which among them are local witnesses for the fact that node satisfies the definition of S. This can be done using algorithms that we proposed in [12] and [19]. For that, neigh(node) is seen as a bag over the alphabet Consumers, by replacing every edge by witness(edge). A bag is an unordered collection with possibly repeated symbols. For instance, the bag...
that corresponds to the mapping \([1,2]\) from Example \([3.1]\) is \([\{\text{TCons}^3_1, \text{TCons}^3_2, \text{TCons}^3_3, \text{TCons}^3_4, \text{TCons}^3_5, \text{TCons}^3_6\}]\). Now, for checking whether a bag belongs to the language of a regular bag expression, we use either the algorithm from \([12]\) based on derivatives of regular expressions, or we use a slight modification of the Interval algorithm presented on Figure 4 in \([19]\). Because the Interval algorithm supports only \([0; 1]\), \([0; \text{unbound}]\), \([1; \text{unbound}]\) repetitions on sub-expressions that are not triple constraints, \(\text{Expr}\) is not a triple constraint: \(\text{Expr}, \text{Expr}, \text{Expr}[0; 1], \text{Expr}[0; 1]\). After the unfolding, we can apply the Interval algorithm.

On the Complexity of Validation. In \([19]\), we showed that validation of SHEx schemas is NP-complete. Note that validation remains in NP with the new constructs defined in the present paper. The high complexity is due to verifying whether the neighbourhood of a node locally satisfies a shape definition. In the algorithm presented here, checking whether a candidate map is a local witness is polynomial if the modified Interval algorithm is used, but there is an exponential number of candidates to be considered (see below). Note also that given \(\text{typing}, \text{lw}\), it is trivial (polynomial) to verify whether this is a global typing witness.

4.3 Implementation and Optimization Guidelines

A first, easily avoidable source of complexity is the computation of \(\text{typing}^\text{cert}, \text{lw}^\text{cert}\), to be fed as input of the flooding algorithm. These can be computed using the algorithm sketched in the proof of Theorem 3.3. An optimized implementation should however compute them on the fly and on demand. This can be performed using a version of the flooding algorithm, for which we give here some guidelines. If a test \((\text{node}, \mathcal{S}) \in \text{typing}^\text{cert}\) or \((\text{node}, \mathcal{S}) \in \text{typing}^\text{cert}\) is required and either \((\text{node}, \mathcal{S})\) or \((\text{node}, \mathcal{S})\) is in the already computed portion of \(\text{typing}^\text{cert}\), we can answer that test right away. If none of the latter has been computed so far, we have to call \(\text{FloodingValidation}\) with \(\text{typing}^\text{cert} = \{(\text{node}, \mathcal{S})\}\). After the call returns, either \((\text{node}, \mathcal{S})\) is in the result typing, then we add it to \(\text{typing}^\text{cert}\), or \(\text{UnchLW}(\text{node}, \mathcal{S})\) is empty, and then we add \((\text{node}, \mathcal{S})\) to \(\text{typing}^\text{cert}\). The function is recursively called if another test involving \(\text{typing}^\text{cert}\) is required during its computation.

Another source of complexity is the computation of \(\text{UnchLW}\); this is also the unique reason for non-tractability of validation. The size of a the set \(\text{CandidateULW}(\text{node}, \mathcal{S})\) can be exponential in the number of repetitions of a property in a shape definition (where extra properties are considered as repetitions). For instance, on the Running Example, the set \(\text{CandidateULW}(\text{node}, \mathcal{S})\) contains \(27 = 3^3\) candidate mappings elements. All these have to be checked as potential elements of \(\text{UnchLW}(\text{node}, \mathcal{S})\). Therefore, decreasing the size of the \(\text{CandidateULW}\) sets is a critical optimization, and can be obtained by decreasing the size of the \(\text{matchingTC}(\text{node})\) sets. For that, we propose to use look-ahead techniques. Continuing on Example \([4]\), the idea is to remove \(\text{TCons}_i\) from \(\text{matchingTC}(\text{edge})\) because \(\text{ex:emin}\), the target node of \(\text{edge}\), does not have a \(\text{isExperience}\), thus cannot satisfy \(<\text{ProgrammerShape}>\) required by \(\text{TCons}_i\). A look-ahead for an edge \(\text{edge} = (\text{node}, q, \text{node})\) and a triple consumer \(\text{TCons}_i\) consists in inspecting only the neighbourhood of \(\text{node}\) trying to prove that \(\text{node}\) does not satisfy some shape \(\mathcal{S}\) that is a conjunct in \(\mathcal{C}_i\), thus allowing to not add \(\text{TCons}_i\) to \(\text{matchingTC}(\text{edge})\).

Finally, the \(\text{UnchLW}\) sets do not need to be stored and can be accessed through an iterator. Every \(\text{CandidateULW}(\text{node}, \mathcal{S})\) is defined as a Cartesian product, so it is easy to iterate on it. On line \(13\) of Algorithm \([2]\), it is enough to retrieve elements from \(\text{CandidateULW}(\text{node}, \mathcal{S})\), through its iterator, until a local witness in \(\text{UnchLW}(\text{node}, \mathcal{S})\) is found.

4.4 Post-Validation Processing

The global typing witness computed by the flooding algorithm associates with every node the shape labels that it satisfies (in \(\text{typing}\)), and with every edge in the neighbourhood of a node, how it participated in satisfying a shape (in \(\text{lw}\)). This allows for post-processing of the graph depending on the “roles” played by the different nodes and edges. For instance, on the Running Example, we could check the additional constraint “all user that reported an issue is affected by that same issue”. Another interesting use case is exporting in e.g. XML format all confirmed issues together with the testers that reproduced them. Exporting in XML and in JSON can be currently performed by two existing modules\([10]\) implemented using semantic actions fired after the validation terminates. Additionally, the global typing witness can be exported using a normalized JSON format\([11]\), thus making post-processing possible using virtually any programming language.

5. ON ERROR IDENTIFICATION

One of the uses of error identification is to guide the user in rendering the input graph into one that is valid i.e., repairing the graph.

Example 5.1 Take the following RDF graph and the schema from the Running Example.

```r
ex:issue:reportedBy ex:emma ;
ex:IssueShape
is:reproducedBy ex:ron, ex:leila .
ex:emma:foaf:name "Emma" ; is:experience is:senior .
ex:ron:foaf:name "Ron" ; is:role is:someRole .
ex:leila:foaf:name "Leila" ; is:experience is:junior ; is:clientNumber 3 ; is:affectedBy ex:issue .
```

The node \(\text{ex:issue}\) does not satisfy \(<\text{IssueShape}>\) because it does not have a property \(\text{is:reproducedBy}\) whose object is a client. One can identify a number of possible scenarios explaining the invalidity of the RDF graph. One is \(\text{ex:emma}\) is missing a \(\text{is:clientNumber}\) property and such should be added. Another is that the triple \(\text{ex:issue}\) is \(\text{reportedBy}\) \(\text{ex:emma}\) uses the wrong property and should be

\[^{9}\text{GenX http://w3.org/brief/NDc1}\]

\[^{10}\text{GenJ http://w3.org/brief/NDc2}\]

\[^{11}\text{GenX http://w3.org/brief/NDc1}\]
replaced by `ex:issue` is:reproducedBy `ex:emma`. Naturally, this would make `ex:issue` not having the required `is:reportedBy` property. To satisfy this requirement two actions are possible: replacing `ex:issue` is:reproducedBy `ex:leila` by `ex:issue` is:reportedBy `ex:leila` since `ex:leila` satisfies `<UserShape>` and `<ClientShape>`, or adding a new node satisfying `<UserShape>` and `<ClientShape>`, and connecting `ex:issue` to the new node with `is:reportedBy`.

Given a schema `Sch`, a graph `G`, and an initial typing `typing₀` of `G` w.r.t. `Sch`, we attempt to find a graph `G'` obtained from `G` with a minimal set of triple insertions and deletions such that `G'` satisfies `S` w.r.t. `typing₀` (replacing the property of an edge consists of deleting and inserting an edge). Basically, we wish to present the user a minimal set of operations that render the input graph valid thus pinpointing possible reasons why `G` is not valid. Such a graph `G'` is called a repair of `G` w.r.t. `Sch`. Unfortunately, the number of different ways of repairing a graph may be (exponentially) large which renders constructing a repair intractable.

**Example 5.2** Take the following instance of RDF

```
<term> ex:has-vars ex:vars .
ex:vars ex:x1-t "x1-true" ; ex:x1-f "x1-false" ;
ex:x2-t "x2-true" ; ex:x2-f "x2-false" .
```

and consider the setting where we wish to verify if the node `ex:term` satisfies the type `<Term>` of the following schema

```
<Term> { ex:has-vars ex:vars }
<Vars> { (ex:x1-t xsd:string | ex:x1-f xsd:string | EmptyShape), (ex:x2-t xsd:string | ex:x2-f xsd:string | EmptyShape) }
```

The repairs of the above RDF instance correspond to the set of all valuations of two Boolean variables `x1` and `x2`, which is extendable to an arbitrary number of variables. Although the schema also permits an empty valuation instance where all the outgoing edges of `ex:vars` are removed, such an instance is not a repair because it is not minimal.

With additional shape definitions in the schema and additional nodes in the RDF graph, one can encode satisfiability of CNF formulas. According to Theorem 5.3 (given here without proof), constructing a repair is unlikely to be polynomial (unless `P=coNP`).

**Theorem 5.3** Checking if a given graph `G'` is a repair of a given graph `G` w.r.t. a given schema `S` and a given initial typing `typing₀` is `coNP`-complete.

Remark that the hardness proof uses only simple schema operators: the some-of operator for encoding disjunction, and the grouping operator for encoding conjunction. Thus, any schema language proposing these or similar operators would have non-tractable repair problem.

Error identification could be approached in a much simpler fashion: rather than repairing the problem just point to the node(s) responsible for the problem and let the user deal with it. This approach is, however, inherently ambiguous as already shown in Example 5.1 and shows the necessity in developing suitable heuristics for error identification.

6. RELATED WORK

**Recursive Validation Language and Cyclic Validation.** In ShEx, a ShapeDefinition has a ShapeExpr composed of TripleConstraints with ValueClasses. In the case that a ValueClass contains a ShapeLabel, the grammar becomes recursive because that ShapeLabel references a ShapeDefinition. For example, an `<IssueShape>` could have an is:related property which references another `<IssueShape>`. If the instance graph has cycles on edges which appear in shapes, validation may arrive at validating the same shape against the same node. The schema languages Description Set Profiles and Resource Shapes described below haven’t considered the problem of detecting or terminating cyclic validation.

**Global Constraints.** Where ShEx focuses on typings of specific instance nodes by shapes, some schema languages define validation for RDF graphs as a whole. This involves some variant of an iteration across nodes in the graph and shapes in the schema to perform a maximal typing. Description Set profiles includes global cardinality constraints describing the number of permissible instances of specified shapes. ShEx’s global maximal typing types all nodes with all the shapes they satisfy.

**Description Set Profiles.** The Dublin Core® Metadata Initiative is developing a constraint language called Description Set Profiles (DSP) [1]. DSP can be represented by an RDF vocabulary and by a conventional XML Schema. DSP has additional value constraints for encoding, language tag lists, and specific rules for subproperties.

DSP does not address repeated properties though a 2008 evaluation of DSP for a “Scholarly Works Application Profile” specifically identified a need for repeated properties e.g. `dc:type`[12] DSP’s current interpretation of repeated properties treats them as conjunctions of constraints. The study found that professional modelers had expected a behavior more like ShEx, i.e. each of the constraints would have to be individually matched by some triples in the neighborhood.

**Resource Shapes.** ShEx was originally created to provide a domain-specific language for Resource Shapes [17]. Resource Shapes is an RDF vocabulary for describing simple conjunctions of shape constraints. While the specification was not clear on this, the author verbally indicated that repeated properties were probably not permitted. Resource Shapes includes descriptive features `oslc:readOnly, oslc:hidden` and `oslc:name` which have no effect on validation but can be useful to tools generating user input forms.

**OWL Based Validation.** Another approach proposed for RDF validation was to use OWL to express constraints. However, the use of Open World and Non-unique name assumption limits validation possibilities. [4][20][14] propose the use of OWL expressions with a Closed World Assump-

http://tinyurl.com/eprint-dc-type1
http://tinyurl.com/eprint-dc-type2
tion to express integrity constraints. The main criticism against such an approach is that it associates an alternative semantics with the existing OWL syntax, which can be misleading for users. Note that in any case, OWL inference engines cannot be used for checking the constraints, and such an approach requires a dedicated implementation.

**SPARQL Based Validation.** It is possible to use SPARQL to express validation constraints although the SPARQL queries can be long and difficult to debug so there is a need for a higher-level language. SPARQL Inferencing Notation (SPIN)\(^9\) constraints associate RDF types or nodes with validation rules. These rules are expressed as SPARQL queries. There have been other proposals using SPARQL combined with other technologies, Simister and Brickley\(^{10}\) propose a combination between SPARQL queries and property paths employed at Google. Kontokostas et al \(^{10}\) proposed **RDF-FUnit** a Test-driven framework which employs SPARQL query templates and Fischer et al \(^{8}\) propose RDF Data Descriptions, a domain-specific language that is compiled into SPARQL queries. SPARQL has much more expressiveness than Shape Expressions and can even be used to validate numerical and statistical computations \(^{11}\). On the other hand, SPARQL does not allow to support recursive constraints and the additive semantics of grouping is difficult to express in SPARQL. Reuter et al \(^{16}\) have recently proposed an extension operator to SPARQL to include recursion. With such operator, it might be possible to compile ShEx to SPARQL.

**SHACL.** The SHACL language is under development and the Working Group has several open issues related to it’s differences with ShEx, most notably Issue 92\(^{11}\) related to the interpretation of repeated properties. While still far from representing consensus in the group, the First Public Working Draft \(^{4}\) includes a core RDF vocabulary similar to but more expressive than Resource Shapes for describing shapes constraints. The other part of the specification includes a SPARQL template convention and an algorithm for iterating through a graph and its constraints. This template system implements the core semantics and, in principle, provides an extensibility mechanism to extend the vocabulary to features which can be verified in atomic SPARQL queries with a supplied subject. Regarding recursion, it is hoped that SHACL will adopt some definition of well-defined schema which will enable sound recursion. To the extend they are defined, SHACL’s AND and OR constructs are analogous to ShEx’s some-of and group (so long as there are no triples in the instance data which could match more than one repeated property). The property constraints attached directly to a SHACL shape appear to have the same behavior as if they were inside an AND construct. There was no schema for SHACL (a so-called SHACL for SHACL) published with the first published working draft. In principle, a sufficiently constraining schema would accept only inputs for which there was a defined semantics. This could provide an anchor for semantic definitions analogous to the role typically performed by an abstract syntax.

7. **CONCLUSIONS AND FUTURE WORK**

ShEx is an expressive schema language for RDF graphs. We illustrated the features of the language with examples, described its semantics, and presented a validation algorithm. ShEx has several open source implementations, and several documentation resources available on the Web. It has been used for the description and the validation of two linked data portals \(^{13}\). ShEx is currently successfully used in medical informatics for describing clinical models. ShEx represents a substantial improvement over contemporary schema languages in features and sound semantics.

As future development of ShEx, we are working on the definition of high-level logical constraints on top of ShEx schemas, on data exchange and data transformation solutions based on ShEx, and on heuristics for helpful error reporting.

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