Extending Shape Expressions for different types of knowledge graphs

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Abstract

Shape Expressions (ShEx) has been proposed as a concise and human-readable language to describe and validate RDF. Inspired by regular expressions, it offers an expressive formalism to describe graph structures based on regular bag expressions. Although plain RDF is one of the common data formats employed to represent knowledge graphs, there have been several proposals to either extend RDF with the so-called RDF-Star or RDF 1.2, or to employ other formalisms like property graphs. In this paper we present an overview and comparison of those approaches and propose three possible extensions of ShEx: ShEx-Star which can be used to validate RDF-Star, ShEx-N: that can be used when nodes also act as properties in RDF and PShEx, which can be used to describe property graphs. We present some examples and a semantics of each extension.

1. Introduction

Although Knowledge graphs have been successfully adopted by the industry, an important aspect of their practical application is the quality of the data that they contain. In order to increase their quality, it is necessary to have some mechanisms that can check the conformance of the data to some kind of schema. Knowledge graphs are usually considered schema-less, because there is no mandatory schema, however, in most cases the data curators have an implicit schema in mind. Having the possibility to materialize that implicit schema into a machine processable form that can be automatically verified can mitigate the risk of non-conformant data.

In practice, there are several types of technologies that can be used for knowledge graphs [1]: Directed edge-labeled graphs, whose main representative are RDF graphs, and Property graphs, which allow property-value pairs and labels to be associated with nodes and edges.

In the case of RDF, two main technologies have been proposed for validation: ShEx [2] and SHACL [3], which are based on the notion of a shape as a description of the topology of some specific kind of nodes. In this way, it is possible to define a schema as a set of shapes which describe the expected properties of some nodes, their expected cardinalities and the kind of nodes. These schemas, can be used to validate RDF data and check if it conforms to those shapes. We employ ShEx in the paper because it can be seen as a description language for RDF acting as grammar where a ShEx schema represents the set of all the RDF graphs that conform to it.

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There has been a proposal for an extension of RDF called RDF-Star [4] and a Working Group is currently working taking that proposal as input to define what is currently called RDF 1.2 [5]. The proposal extends RDF with the possibility of having triples as subjects or objects in statements. The relationship between that extension and property graphs has already been studied [6].

Although ShEx was defined to describe and validate RDF, we consider that it can be extended to describe and validate RDF-Star (or RDF 1.2), so in this paper we explore a possible extension of the language in that direction. Apart from that, the shapes in ShEx are usually centered on describing nodes that act as either subjects or objects, but in RDF, it is also possible to add statements whose subjects or objects are also the predicates of other statements. We also explore a possible extension of ShEx where it is possible to define shapes about nodes that act as properties. Finally, although there have been several proposals to define schemas for property graphs, we consider that the grammar-based approach of ShEx can also be helpful, so we also explore what it would look like to extend ShEx for describing and validating property graphs.

The main contributions of this paper are to present three extensions of ShEx: ShEx-Star for RDF-Star (section 3), ShEx-N for describing nodes as properties (section 4) and PShEx for property graphs (section 5), with their abstract syntax and semantic definitions.

2. RDF and ShEx

Definition 1 (RDF triple and RDF Graph). Given a set of IRIs I, a set of blank nodes B and a set of literals Lit, an RDF triple is a tuple (s, p, o) where $s \in I \cup B$ is called the subject, $p \in I$ is called the predicate and $o \in I \cup B \cup Lit$ is called the object. An RDF graph G is a set of RDF triples.

There are several syntaxes for RDF graphs like Turtle, N3, RDF/XML, etc. In this document, we will use Turtle.

Example 1 (Example of an RDF graph in Turtle). The following snippet contains a simple RDF graph with two nodes : a and : b.

```
prefix : <http://example.org/>
:a :name "Alice" ;
    :knows :b .
:b :firstname "Robert", "Julius" ;
    :lastname "Smith" .
```

The neighbors of a node $n \in V$ in an RDF graph G are defined as $neighs(n,G) = \{(n,p,y) \mid (n,p,y) \in G\} \cup \{(x,p,n) \mid (x,p,n) \in G\} \cup \{(x,n,y) \mid (x,n,y) \in G\}.$

Shape Expressions (ShEx) were proposed as such a language in 2014 [2]. It was designed as a high-level and concise domain-specific language to describe RDF. The syntax of ShEx is inspired

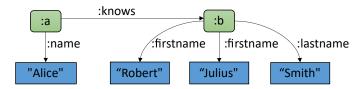


Figure 1: Basic RDF graph example

by Turtle and SPARQL, while the semantics was inspired by RelaxNG and XML Schema. In this section we describe a simplified abstract syntax of ShEx following [8]¹.

Definition 2 (ShEx schema). A *ShEx Schema* is defined as a tuple $\langle L, \delta \rangle$ where L is the set of shape labels, and $\delta : L \to S$ is a total function from labels to shape expressions. The set of shape expressions $se \in S$ is defined using the following abstract syntax:

```
se ::=
           cond
                            Basic boolean condition on nodes (node constraint)
                            Conjunction of se_1 and se_2
           se_1 and se_2
                            Shape label reference for l \in L
           @l
           CLOSED \{te\}
                            Closed shape
                            Open shape
           \{te\}
te
          te_1; te_2
                            Each of te_1 and te_2
           te_1 \mid te_2
                            Either te_1 or te_2
           te*
                            Zero or more te
           \ \ \overset{p}{\hookrightarrow} se
                            Outgoing Triple with predicate p and object conforming to se
                            Incoming triple with predicate p and subject conforming to se
                            Empty triple expression
```

Intuitively, shape expressions define conditions about nodes while triple expressions define conditions about the neighborhood of nodes, and shapes qualify those neighborhoods by allowing (open shapes) or disallowing (closed shapes) triples with other predicates. We omit negation and disjunction operator to simplify the interactions between negation and recursion, which led to a stratified negation requirement in ShEx.

The restrictions imposed on shape expressions schemas in [9] also apply here. Namely, in a schema (L, δ, S)

- The shape label references used by the definition function δ are themselves defined, i.e. if @l appears in some shape definition, then l belongs to L;
- No definition $\delta(l)$ uses a reference @l to itself, neither directly nor transitively, except while traversing a shape. For instance, $\delta(l) = @l$ and se is forbidden, but $\delta(l) = \{ \bot \stackrel{p}{\to} @l \}$ is allowed.

Example 2 (Example of ShEx schema). A ShEx schema that describes the RDF graph presented in example 1 can be defined as:

¹The full specification of ShEx is available at https://shex.io/shex-semantics/

ShEx has several concrete syntaxes like a compact syntax (ShExC) and an RDF syntax defined based on JSON-LD (ShExJ) 2 .

Example 3. An example of a ShEx schema using ShExC compact syntax.

```
prefix : <http://example.org/>
prefix xsd: <http://www.w3.org/2001/XMLSchema#>
<Person> {
  (:name xsd:string |
    :firstname xsd:string * ; :lastname xsd:string );
    :knows @<Person> *
}
```

The semantics of ShEx schemas is based on a conformance relation parameterized by a shape assignment: we say that node n in graph G conforms to shape expression se with shape assignment τ , and we write $G, n, \tau \models se$.

The following rules are defined similar to [10], where it is shown that there exists a unique maximal shape assignment $\tau_{\rm max}$ that allows us to define conformance independently of the shape assignment. The conformance relation is defined recursively on the structure of se by the set of inference rules presented in table 1 where preds(te) is the set of predicates that appear in a triple expression te and can be defined as:

$$Cond\frac{cond(n) = true}{G, n, \tau \vDash cond} \qquad AND \frac{G, n, \tau \vDash se_1 \quad G, n, \tau \vDash se_2}{G, n, \tau \vDash se_1 \quad AND \quad se_2}$$

$$ShapeRef \frac{\delta(l) = se \quad G, n, \tau \vDash se}{G, n, \tau \vDash @l} \qquad ClosedShape \frac{neighs(n, G) = ts \quad G, ts, \tau \vDash te}{G, n, \tau \vDash \textbf{closed} \ \{te\}}$$

$$OpenShape \frac{ts = \{\langle x, p, y \rangle \in neighs(n, G) \mid p \in preds(te)\} \quad G, ts, \tau \vDash te}{G, n, \tau \vDash \{te\}}$$

Table 1Inference rules for ShEx shape expressions

```
\begin{array}{lll} preds(te_1;te_2) & = & preds(te_1) \cup preds(te_2) \\ preds(te_1 \mid te_2) & = & preds(te_1) \cup preds(te_2) \\ preds( \xrightarrow{p} te) & = & \{p\} \\ preds(te*) & = & preds(te) \\ preds(\epsilon) & = & \emptyset \end{array}
```

²See ShEx specification [9] for details.

The rules for node constraints (Cond) and conjunction are as expected. A node n conforms to an open shape with triple expression te if its neighborhood restricted to the triples with predicates from te conform, meaning that triples whose predicates are not mentioned in te are not constrained by the shape (rule OpenShape). Conformance to a closed shape requires to consider the whole neighborhood of the node (rule ClosedShape).

Conformance to a triple expression uses a second relation defined on sets on neighborhood triples ts instead of nodes n. The set of neighborhood nodes ts of a graph G conforms to a triple expression te with shape assignment τ , written as $G, ts, \tau \Vdash te$, as defined by the inference rules in table 2.

$$EachOf \frac{(ts_{1},ts_{2}) \in part(ts)}{G,ts,\tau \Vdash te_{1}} \frac{G,ts_{2},\tau \Vdash te_{2}}{G,ts,\tau \Vdash te_{1};te_{2}}$$

$$OneOf_{1} \frac{G,ts,\tau \Vdash te_{1}}{G,ts,\tau \Vdash te_{1} \mid te_{2}} \qquad OneOf_{2} \frac{G,ts,\tau \Vdash te_{2}}{G,ts,\tau \Vdash te_{1} \mid te_{2}}$$

$$TC_{1} \frac{ts = \{\langle x,p,y \rangle\} \quad G,y,\tau \vdash se}{G,ts,\tau \Vdash \Box \stackrel{p}{\rightarrow} se} \qquad TC_{2} \frac{ts = \{\langle y,p,x \rangle\} \quad G,y,\tau \vdash se}{G,ts,\tau \Vdash se \stackrel{p}{\rightarrow} \Box}$$

$$Star_{2} \frac{(ts_{1},ts_{2}) \in part(ts) \quad G,ts_{1},\tau \Vdash te}{G,ts,\tau \Vdash te*} \qquad Star_{1} \frac{G,\emptyset,\tau \Vdash te*}{G,\emptyset,\tau \Vdash te*}$$

Table 2
Inference rules for ShEx triple expressions

A shape assignment τ for graph G and S is called *valid* if for every node n in G and every shape expression label l defined in S, if $n@l \in \tau$, then $G, n, \tau \models @l$.

According to Boneva et al [8], for every graph G, there exists a unique maximal valid shape assignment τ_{\max} such that if τ is a valid shape assignment for G and S, then $\tau \subseteq \tau_{\max}$.

3. RDF-Star and ShEx-Star

RDF-Star has been proposed as an extension of RDF where the subjects and objects can be triples. We present a formal definition of RDF-Star based on [11]:

Definition 3 (RDF-Star). An RDF-Star triple is a tuple t defined recursively as follows: Any RDF triple $t \in (I \cup B) \times I \times (I \cup B \cup Lit)$ is an RDF-Star triple; and given RDF-Star triples t and t' and RDF terms $s \in (I \cup B)$, $p \in I$ and $o \in (I \cup B \cup Lit)$, the tuples $(\ll t \gg, p, o)$, $(s, p, \ll t' \gg)$ and $(\ll t \gg, p, \ll t' \gg)$ are RDF-Star triples. An RDF-Star graph is a set of RDF-Star triples.

Example 4 (Example of an RDF-Star graph in Turtle-Star notation). The following snippet contains a simple RDF-Star graph with two nodes: a and: b.

```
prefix : <http://example.org/>
```

```
:a :name "Alice" .
<< :a :knows :b >> :certainty 0.5 .
:b :firstname "Robert", "Julius" ;
    :lastname "Smith" .
```

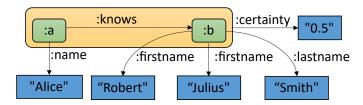


Figure 2: Basic RDF-Star example

We can extend ShEx to support ShEx-Star by adding the following declaration to the definition of triple expressions te:

Example 5 (Example of a ShEx-Star schema). A ShEx-Star schema that describes the RDF graph presented in example 4 can be defined as:

$$\delta(Person) = \{ (_ \xrightarrow{name} String | _ \xrightarrow{fistname} String^*; _ \xrightarrow{lastname} String); \\ \ll _ \xrightarrow{knows} @Person \gg \{|_ \xrightarrow{certainty} Decimal|\}^* \}$$

The expression $\ll \Box \stackrel{p}{\to} se \gg \{|te|\}$ describes a triple term whose predicate is p and whose object conforms to the shape expression se and that can be the subject of triples conforming to triple expression te. The formal semantics can be described as:

$$TTC_{1} \cfrac{ts = \{\langle \ll t \gg, p, y \rangle\} \qquad G, y, \tau \vDash se \quad neighs(\ll t \gg, G) = ts' \qquad G, ts', \tau \Vdash te}{G, ts, \tau \Vdash \ll \Box \xrightarrow{p} se \gg \{|te|\}}$$

$$TTC_{2} \cfrac{ts = \{\langle x, p, \ll t \gg \rangle\} \qquad G, x, \tau \vDash se \quad neighs(\ll t \gg, G) = ts' \qquad G, ts', \tau \Vdash te}{G, ts, \tau \Vdash \ll se \xrightarrow{p} \Box \gg \{|te|\}}$$

Table 3Inference rules for ShEx-Star new triple term expressions

4. ShEx-N: Describing nodes that act as properties

In the RDF data model, predicates can also act as subjects or objects or triples. This aspect is not taken into account in traditional ShEx, where the shapes describe the topology of nodes without considering their potential role as predicates.

Example 6 (Example of an RDF graph a node acting as a property). The following snippet contains a simple RDF graph where : knows is both a node and a property.

```
prefix : <http://example.org/>
prefix skos: <http://www.w3.org/2004/02/skos/core#>

:a :name "Alice" ;
    :knows :b .
:b :firstname "Robert", "Julius" ;
    :lastname "Smith" .
:knows skos:related :Friendship .
```

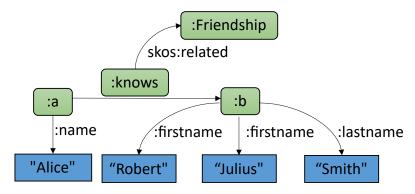


Figure 3: RDF example with a property as a node

In order to capture these appearances in a single shape, it is possible to add a new kind of triple expression:

```
te ::= \ldots Same definitions as in 2 |se_1 \xrightarrow{\smile} se_2  Triple constraint with focus node acting as predicate and subject conforming to se_1 and object conforming to se_2
```

The semantics of triple term constraints can be defined as:

$$NP_1 \frac{ts = \{\langle s, x, o \rangle\} \quad G, s, \tau \vDash se_1 \quad G, o, \tau \vDash se_2}{G, ts, \tau \Vdash se_1 \quad \stackrel{\rightharpoonup}{\hookrightarrow} se_2}$$

Table 4 Inference rules for ShEx-N

Example 7 (Example of a ShEx-N schema). The following ShEx-N schema defines the shape *FrienshipProperty* which validates the node :knows in example 6:

5. Property graphs and PShEx

Property graphs have become popular thanks to several commercial graph databases like Neo4j ³, JanusGraph ⁴ or Sparksee ⁵. A property graph has unique identifiers for each node/edge and allows to add property-value annotations to each node/edge in the arc as well as type annotations. The following definition of a property graph follows [12].

Definition 4 (Property graph). Given a set of types T, a set of properties P, and a set of values V, a property graph G is a tuple $\langle N, E, \rho, \lambda_n, \lambda_e, \sigma \rangle$ where $N \cap E = \emptyset$, $\rho : E \mapsto N \times N$ is a total function, $\lambda_n : N \mapsto FinSet(T)$, $\lambda_e : E \mapsto T$, and $\sigma : N \cup E \times P \mapsto FinSet(V)$.

A property graph is formed by a set of node identifiers N and a set of edges E where ρ associates a pair of nodes (n_1,n_2) to every $e \in E$ where n_1 is the subject and n_2 is the object, λ_n associates a set of types for node identifiers (notice that property graphs allow nodes to have more than one type), λ_e associates a types for each edge identifier, and σ associates a set of values to pairs (i,p) such that $i \in N \cup E$ is a node or edge and $p \in P$ is a property.

Example 8. As an example, we will represent information that Alice knows Robert with a certainty of 0.5

```
\begin{split} T &= \{ \text{Person, knows} \} \quad P &= \{ \text{name, certainty} \} \quad V = \{ \text{"Alice", "Robert", "Julius", "Smith", 0.5} \} \\ N &= \{ n_1, n_2 \} \quad E &= \{ r_1 \} \quad \rho = r_1 \mapsto (n_1, n_2) \\ \lambda_n &= n_1 \mapsto \{ \text{Person} \}, \; n_2 \mapsto \{ \text{Person} \} \quad \lambda_e = r_1 \mapsto \text{knows} \\ \sigma &= (n_1, name) \mapsto \{ \text{"Alice"} \} \quad (n_2, firstname) \mapsto \{ \text{"Robert", "Julius"} \} \\ (n_2, lastname) \mapsto \{ \text{"Smith"} \} \quad (r_1, certainty) \mapsto \{ 0.5 \} \end{split}
```

Figure 4 presents a possible visualization of a property graph.

We define a ShEx extension called PShEx that can be used to describe and validate Property graphs. In property graphs, nodes and edges can have associated labels as well as a set of property/values. In this way, it is necessary to adapt the definition of ShEx to describe pairs or property/values. PShEx is composed of three main categories: shape expressions (se) that describe the shape of nodes, triple expressions (te) that describe the shape of edge relationships

³https://neo4j.com/

⁴https://janusgraph.org/

⁵https://www.sparsity-technologies.com/#sparksee

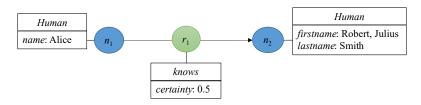


Figure 4: Example graph visualization of a property graph

and property-value expressions (pvs) that describe sets of property/values associated with node/edge identifiers.

Definition 5 (PShEx schema). A *PShEx Schema* is a tuple $\langle L, \delta \rangle$ where L set of shape labels, and $\delta: L \to S$ is a total function from labels to shape expressions $se \in S$ defined using the abstract syntax:

```
Basic boolean condition on set of types t_s \subseteq T
se
       ::=
            cond_{t_s}
                              Conjunction
            se_1 and se_2
                             Shape label reference for l \in L
            @l
            pvs
                             Property-value specifiers of a node
            CLOSED \{te\}
                             Closed shape
            \{te\}
                              Open shape
te
       := te_1; te_2
                             Each of te_1 and te_2
            te_1 \mid te_2
                             Some of te_1 or te_2
            te*
                             Zero or more te
             \square \xrightarrow{p} @l \ pvs
                             Triple constraint with property type p
                             whose nodes satisfy the shape l and property-values pvs
                             Open property-value specifiers ps
pvs
            |ps|
            \lceil ps \rceil
                             Closed property-value specifiers ps
ps
                             Each of ps_1 and ps_2
            ps_1, ps_2
            ps_1 \mid ps_2
                             OneOf of ps_1 or ps_2
                             zero of more ps
                             Property p with value conforming to cond_v
                             cond_{v_s} is a boolean condition on sets of values v_s \subseteq V
```

Example 9. As an example, we can define a PShEx schema that describes the property graph from example 8 where $hasType_t$ is a condition that is satisfied when the set of types of a node contains the type t, i.e. $hasType_t(vs) = \texttt{true}$ if $t \in vs$ and String, Decimal are conditions on the values that are satisfied when the values have the corresponding type.

```
\begin{array}{lll} L & = & \{ \textit{Person} \} \\ \delta(\textit{Person}) & = & \textit{hasType}_{\textit{Human}} \, \textbf{and} \\ & & \lfloor \textit{name} : \textit{String} \mid \textit{firstname} : \textit{String} * , \textit{lastname} : \textit{String} \rfloor \, \textbf{and} \\ & \{ \_ \, \frac{\textit{knows}}{} \, @\textit{Person} \mid \textit{certainty} : \textit{Decimal} \, |^* \} \end{array}
```

In order to define the semantic specification of PShEx we will need to define the neighborhood of a node in a property graph.

The neighbors of a node $n \in N$ in a property graph $G = \langle N, E, \rho, \lambda_n, \lambda_e, \sigma \rangle$ are defined as $neighs(n) = \{(n, p, y, vs) \mid \exists v \in E \text{ such that } \rho(v) = (n, y) \land \lambda_e(v) = p \land vs = \{(k, v) \mid \exists v \in E \text{ such that } \rho(v) = v \land vs = \{(k, v) \mid \exists v \in E \text{ such that } \rho(v) = v \land vs = \{(k, v) \mid \exists v \in E \text{ such that } \rho(v) = v \land vs = \{(k, v) \mid \exists v \in E \text{ such that } \rho(v) = v \land vs = \{(k, v) \mid \exists v \in E \text{ such that } \rho(v) = v \land vs = \{(k, v) \mid \exists v \in E \text{ such that } \rho(v) = v \land vs = \{(k, v) \mid \exists v \in E \text{ such that } \rho(v) = v \land vs = \{(k, v) \mid \exists v \in E \text{ such that } \rho(v) = v \land vs = \{(k, v) \mid \exists v \in E \text{ such that } \rho(v) = v \land vs = \{(k, v) \mid \exists v \in E \text{ such that } \rho(v) = v \land vs = \{(k, v) \mid \exists v \in E \text{ such that } \rho(v) = v \land vs = \{(k, v) \mid \exists v \in E \text{ such that } \rho(v) = v \land vs = \{(k, v) \mid \exists v \in E \text{ such that } \rho(v) = v \land vs = \{(k, v) \mid \exists v \in E \text{ such that } \rho(v) = v \land vs = \{(k, v) \mid \exists v \in E \text{ such that } \rho(v) = v \land vs = \{(k, v) \mid \exists v \in E \text{ such that } \rho(v) = v \land vs = \{(k, v) \mid \exists v \in E \text{ such that } \rho(v) = v \land vs = \{(k, v) \mid \exists v \in E \text{ such that } \rho(v) = v \land vs = \{(k, v) \mid \exists v \in E \text{ such that } \rho(v) = v \land vs = \{(k, v) \mid \exists v \in E \text{ such that } \rho(v) = v \land vs = \{(k, v) \mid \exists v \in E \text{ such that } \rho(v) = v \land vs = \{(k, v) \mid v \in E \text{ such that } \rho(v) = v \land vs = \{(k, v) \mid v \in E \text{ such that } \rho(v) = v \land vs = \{(k, v) \mid v \in E \text{ such that } \rho(v) = v \land vs = \{(k, v) \mid v \in E \text{ such that } \rho(v) = v \land vs = \{(k, v) \mid v \in E \text{ such that } \rho(v) = v \land vs = \{(k, v) \mid v \in E \text{ such that } \rho(v) = v \land vs = \{(k, v) \mid v \in E \text{ such that } \rho(v) = v \land vs = \{(k, v) \mid v \in E \text{ such that } \rho(v) = v \land vs = \{(k, v) \mid v \in E \text{ such that } \rho(v) = v \land vs = \{(k, v) \mid v \in E \text{ such that } \rho(v) = v \land vs = \{(k, v) \mid v \in E \text{ such that } \rho(v) = v \land vs = \{(k, v) \mid v \in E \text{ such that } \rho(v) = v \land vs = \{(k, v) \mid v \in E \text{ such that } \rho(v) = v \land vs = \{(k, v) \mid v \in E \text{ such that } \rho(v) = v \land vs = \{(k, v) \mid v \in E \text{ such that } \rho(v) = v \land vs = \{(k, v) \mid v \in E \text{ such that } \rho(v) = v \land vs = \{(k, v) \mid v \in E \text{ such that } \rho(v) = v \land vs = \{(k, v) \mid v \in E \text{ such that } \rho$

 $\sigma(k,v)=ws \wedge v \in ws\}$. For a node n, we define the property value set as $propvs(n)=\{(k,v)\mid \sigma(k,v)=ws \wedge v \in ws\}$

The semantic specification of PShEx can be defined in a similar way to the ShEx one. Given a property graph G, and a shape assignment τ , a node identifier $n \in N$ conforms with a shape expression se, which is represented as $G, n, \tau \models se$ and follows the rules presented in 5 where preds(te) is the set of edge labels (or predicates) that appear in a triple expression te and can be defined as:

$$Cond_{ts} \cfrac{\lambda_n(n) = vs \quad cond_{ts}(vs) = true}{G, n, \tau \models cond_{ts}} \qquad AND \cfrac{G, n, \tau \models se_1 \quad G, n, \tau \models se_2}{G, n, \tau \models se_1 \text{ AND } se_2}$$

$$ClosedShape \cfrac{neighs(n, G) = ts \quad G, ts, \tau \Vdash s'}{G, n, \tau \models \textbf{closed}} \{te\}$$

$$OpenShape \cfrac{ts = \{\langle x, p, y \rangle \in neighs(n, G) \mid p \in preds(te)\} \quad G, ts, \tau \Vdash te}{G, n, \tau \models \{te\}}$$

$$ShapeRef \cfrac{\delta(l) = se \quad G, n, \tau \models se}{G, n, \tau \models se} \qquad PVS \cfrac{propvs(n) = s \quad G, s, \tau \vdash pvs}{G, n, \tau \models pvs}$$

Table 5Rules for PShEx shape expressions

```
\begin{array}{lll} preds(te_1;te_2) & = & preds(te_1) \cup preds(te_2) \\ preds(te_1 \mid te_2) & = & preds(te_1) \cup preds(te_2) \\ preds(\_ \xrightarrow{p} te) & = & \{p\} \\ preds(te*) & = & preds(te) \\ preds(\epsilon) & = & \emptyset \end{array}
```

As in the case of ShEx, the previous definition uses a second conformance relation defined on sets of triples ts instead of nodes n. The set of neighborhood nodes ts from a property graph G conforms to a triple expression te with shape assignment τ , written $G, ts, \tau \Vdash s$, as defined by the inference rules represented in table 6.

In the case of PShEx we declare a new conformance relationship $G, s, \tau \vdash qs$ between a graph G a set $s \in P \times V$ of property-value elements, a shape assignment τ and a property-value specifier pvs whose rules are defined in table 7 where props(pvs) is the set of properties that appear in a property-value specifier ps and can be defined as:

```
\begin{array}{lll} props(ps_1\,,\,ps_2) &=& props(ps_1) \cup props(ps_2) \\ props(ps_1 \mid ps_2) &=& props(ps_1) \cup props(ps_2) \\ props(ps*) &=& preds(ps) \\ props(p:cond_v) &=& \{p\} \end{array}
```

As in the case of ShEx, the semantics of ShEx schemas can be defined independently on shape assignments. A shape assignment τ for graph G and S is called *valid* if for every node n in G and every shape expression label l defined in S, if $n@l \in \tau$, then $G, n, \tau \models @l$.

$$EachOf \frac{(ts_{1},ts_{2}) \in part(ts) \quad G,ts_{1},\tau \Vdash te_{1} \quad G,ts_{2},\tau \Vdash te_{2}}{G,ts,\tau \Vdash te_{1};te_{2}}$$

$$OneOf_{1} \frac{G,ts,\tau \Vdash te_{1}}{G,ts,\tau \Vdash te_{1} \mid te_{2}} \quad OneOf_{2} \frac{G,ts,\tau \Vdash te_{2}}{G,ts,\tau \Vdash te_{1} \mid te_{2}}$$

$$TripleConstraint \frac{ts = \{\langle x,p,y,s \rangle\} \quad G,y,\tau \vDash @l \quad G,s,\tau \vdash qs}{G,ts,\tau \Vdash te^{2}} \frac{G,ts,\tau \vdash te_{2}}{G,ts,\tau \vdash te^{2}}$$

$$Star_{1} \frac{G,\emptyset,\tau \vdash te^{2}}{G,ts,\tau \vdash te^{2}}$$

$$Star_{2} \frac{(ts_{1},ts_{2}) \in part(ts) \quad G,ts_{1},\tau \vdash te \quad G,ts_{2},\tau \vdash te^{2}}{G,ts,\tau \vdash te^{2}}$$

Table 6Rules for PShEx triple expressions

$$OpenPVs = \frac{s' = \{(p,v) \in s | p \in props(ps)\} \quad G, s', \tau \vdash ps}{G, s, \tau \vdash [ps]} \qquad ClosePVs = \frac{G, s, \tau \vdash ps}{G, s, \tau \vdash [ps]}$$

$$EachOfPs = \frac{G, s, \tau \vdash ps_1 \quad G, s, \tau \vdash ps_2}{G, s, \tau \vdash ps_1, ps_2}$$

$$OneOfPs_1 = \frac{G, s, \tau \vdash ps_1}{G, s, \tau \vdash ps_1 \mid ps_2} \qquad OneOfPs_2 = \frac{G, s, \tau \vdash ps_2}{G, s, \tau \vdash ps_1 \mid ps_2}$$

$$StarPs_1 = \frac{(s_1, s_2) \in part(s) \quad G, s_1, \tau \vdash ps}{G, s, \tau \vdash ps*} = \frac{G, s_2, \tau \vdash ps*}{G, s, \tau \vdash ps*}$$

$$PropertyValue = \frac{s = \{(p, w)\} \quad conv_v(w) = \mathbf{true}}{G, s, \tau \vdash p : cond_v}$$

Table 7Rules for PShEx property-value specifiers

6. Related work

ShEx was initially proposed in 2014 [2] as a concise and human readable language to describe and validate RDF. It was based on a variant of regular expressions called Regular Bag Expressions [13] which also supports recursive shapes. Combining negation with recursive shapes was later studied in [10] where a well founded formal semantics for ShEx for proposed based on stratification. Our definition of ShEx is based on that work, although we omitted negation, disjunction and EXTRA declarations of shape expressions in this paper. After ShEx was proposed, a W3C Data Shapes working group was chatered whose result was SHACL, proposed as a recommendation in 2017 [3]. The specification of SHACL didn't have an abstract syntax and left the semantics of recursive shapes as an implementation dependent feature enabling the appearance of several proposals that define an abstract syntax and add semantics for SHACL with negation and recursion [14, 15, 16, 17]. A comparison between both ShEx and SHACL was

provided in [18] while in [19], a simple language was defined that can be used as a common subset of both. We consider that some of our extensions to ShEx could also be applied to SHACL.

The approach followed in this paper to extend ShEx was started in this paper [20] where we had already proposed an initial version of PShEx and WShEx [21], another extension of ShEx to support the Wikibase data model. WShEx is conceptually similar to PShEx although a distinct feature of the Wikidbase data model is that the values of properties can also be nodes in the graph, which can be considered as a generalized property graphs model. This model was called MARS (Multi-Attributed Relational Structures) in [22].

There are several proposals for property graphs schemas. GQL is an upcoming ISO standard (ISO39075) ⁶ which is currently being developed and addresses the property graph model. In order to provide support for GQL, PG-Schema [23] was proposed as a simple schema language for property graphs. PG-Schema does not support cardinality constraints on edges, which could be simulated using PG-Keys [27]. In [24], the authors propose a common framework for property graph schema languages based on first order logic rules which supports cardinality constraints. The closest proposal to PShEx would be the Property Graph Shapes Language (ProGS) [12] although that language is based on SHACL and some of the differences SHACL vs ShEx could also be applied to ProGS vs PShEx. For example, PShEx doesn't have property path expressions and ProGS doesn't have regular bag expressions. Another difference is that ProGS includes negation and recursion while in the version of PShEx included in this paper we omitted negation. Comparison between RDF-Star and property graphs at the data model have already been studied. In [25] proposes a common model for RDF, RDF-Star and property graphs that they call statement graph, which is inspired by the OneGraph [26] vision. The conversion between property graphs and RDF/RDF-Star is also studied in [6].

7. Conclusions and future work

We have presented three extensions to ShEx for different types of knowledge graphs: ShEx-* adds support for RDF-Star, ShEx-N adds a constraint to describe nodes that act as properties, and PShEx can be used to describe and validate property graphs. We presented an abstract syntax and formal semantics for each of the variants.

There are several lines of future work. On the theoretical level, it will be necessary to research the computational complexity implications of these features as well as the combination of these features with other features from ShEx like negation, disjunction, EXTRA declarations, and even the potential integration of all the features together in a single language. On the implementation level: it will be necessary to propose a concrete compact syntax for each variant that can be useful by data model engineers as well as devise algorithms that can be used to check the conformance of graphs to the corresponding schemas. Although we used ShEx in this paper, another line of future work would be to check which of the features proposed in this paper could also be applied to SHACL.

⁶https://www.iso.org/standard/76120.html

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