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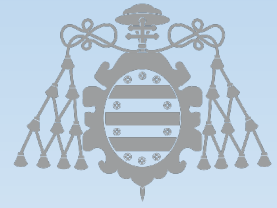
Trabajo de investigación

Plaza F036-570-DFA0340

Área de Lenguajes y Sistemas Informáticos

Departamento de Informática

Jose Emilio Labra Gayo

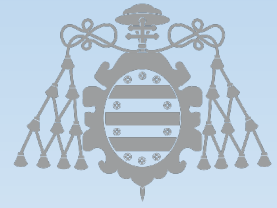


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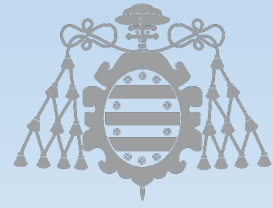
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1. Introducción

Este documento contiene el trabajo de investigación realizado por el candidato Jose Emilio Labra Gayo para la plaza de Catedrático de Universidad número 16, convocada por la Universidad de Oviedo en la Resolución de 25 de Junio de 2021, (BOE de 9 de Julio de 2021), con el código F036-570-DFA0340 del Cuerpo de *Catedrático de Universidad*, para el área de conocimiento *Lenguajes y Sistemas Informáticos*.



2. Contexto del trabajo de investigación

El presente trabajo de investigación se enmarca dentro de la línea de investigación llevada a cabo por el candidato en los últimos años dentro del grupo de investigación WESO.

2.1 Justificación de la temática

Se ha escogido como temática para el trabajo de investigación la creación de subconjuntos de grafos de conocimiento mediante Shape Expressions por varios motivos:

- La implicación del candidato en la creación del lenguaje Shape Expressions y sus diferentes aplicaciones. Mediante el presente trabajo se ahonda en una nueva aplicación de Shape Expressions como lenguaje para describir y extraer subconjuntos de Wikidata.
- Puede resolver un problema práctico real que consiste en poder consumir datos de grandes grafos de conocimiento. Actualmente, Wikidata podría decirse que corre el peligro de morir de éxito al aumentar continuamente la cantidad de datos que almacena. Esta gran cantidad de información ofrece una herramienta muy potente, pero tiene el problema de que es difícil para un usuario convencional poder consumir estos datos. La posible existencia de un sistema que permita crear una instantánea de los datos existentes en Wikidata en un determinado dominio y extraerlos de forma fácil para poder integrarlos con otras aplicaciones se ha convertido en una gran demanda por la comunidad de usuarios.
- La participación del candidato como coordinador en varios eventos cuya temática era la creación de subconjuntos de grafos de conocimiento. En concreto:
 - Hackathon virtual asociado al congreso SWAT4(HC)LS 2020 que se celebra en Enero de 2021 y en el que se continúa trabajando en la creación de técnicas de creación y gestión de subconjuntos de Wikidata¹.
 - Biohackathon Europe, 2020. Evento que se celebró de forma virtual y que fue liderado por el candidato. La actividad realizada durante el evento dará lugar a las publicaciones [30, 38]. En dicho evento se identifican varios casos de uso como el proyecto GeneWiki o Scholia, y se consigue generar subconjuntos de Wikidata mediante WDum-

¹https://swat4hcls.wiki.opencura.com/wiki/Main_Page

per y la técnica ShEx+Slurping.

- En el Biohackathon realizado en Fukuoka, Japón, se entra en contacto con Leyla Garcia y Egon Willighagen, entre otros, participando en la presentación de diversas aplicaciones de Shape Expressions. Algunas de las tareas llevadas a cabo en dicho Biohackathon se publicaron en [9]
- En el hackathon SWAT4(HC)LS de 2019 se comienza a plantear la posibilidad de desarrollar herramientas para la creación de subconjuntos de Wikidata.
- El creciente interés en la utilización de grafos de conocimiento, especialmente Wikidata y la involucración del candidato en la comunidad de Wikidata, participando en varios eventos como la Conferencia de Wikidata (WikidataCon) de 2019 y el Wikimedia Hackathon de Praga de 2019. La adopción por parte de Wikidata de esquemas de entidades basados en el lenguaje ShEx suponen la creación de numerosos esquemas para diferentes dominios² que podrán utilizarse para la generación de subconjuntos.
- La subcontratación durante el verano de 2021 del equipo WESO por parte de la Universidad de Virginia para la realización de un prototipo que mejorase el proyecto Scholia, que incluía como tarea la utilización de subconjuntos de Wikidata en el ámbito de Scholia
- Ha sido motivo de interés de Andra Waagmeester y el proyecto GeneWiki [8] la necesidad de creación de subconjuntos relacionados con la información existente en Wikidata sobre enfermedades, tratamientos, medicinas, genes, etc. De hecho, actualmente ya se está colaborando con los miembros de dicho equipo en el análisis y gestión de los primeros subconjuntos de datos generados.
- La concesión del proyecto ANGLIRU en la convocatoria Retos del Plan Nacional de Investigación, que incluye precisamente, como uno de los entregables, la creación de herramientas para la generación de subconjuntos de grafos de conocimiento.
- Puede suponer un avance en la disciplina, dado que se intenta resolver uno de los problemas existentes hoy en día en la Web Semántica, que es mejorar el consumo de datos semánticos, que se espera que redunde en un mayor uso de estas técnicas y a la postre, permita mejorar el acceso al conocimiento.

Los motivos anteriores han servido de aliciente al candidato para involucrarse en los últimos meses en la temática del trabajo de investigación, lo cual ha consistido en realizar el trabajo teórico plasmado en el artículo que se presenta e implementar prototipos de los algoritmos en las librerías WDSUB y SparkWDSUB usando el lenguaje Scala.

2.2 Formato del trabajo de investigación

En el Reglamento para los concursos de acceso a los cuerpos de funcionarios docentes universitarios de la Universidad de Oviedo, aprobado por el Consejo de Gobierno de 18 de diciembre de 2008 (Boletín Oficial del Principado de Asturias de 14 de enero de 2009) se indica que para la segunda prueba del concurso, el candidato debe presentar un resumen de su trabajo de investigación, sin especificar el formato ni el idioma del mismo.

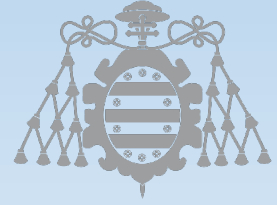
Se ha considerado conveniente presentar el trabajo de investigación con la estructura de un artículo científico extendido y se ha publicado como un *preprint* en el repositorio Arxiv³.

Una vez finalizado el concurso, será enviado para su posible publicación a un congreso o revista de investigación que todavía no ha sido seleccionado.

Por ese motivo, el artículo se presenta en idioma inglés dado que en la convocatoria no se hace mención explícita a requisitos de idioma.

²https://www.wikidata.org/wiki/Wikidata:Database_reports/EntitySchema_directory

³<https://arxiv.org/>



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3. Resumen trabajo de investigación

Creating Knowledge Graph Subsets using Shape Expressions

Jose Emilio Labra Gayo

3.1 Abstract

The initial adoption of knowledge graphs by Google and later by big companies has increased their popularity. In this paper we present a formal model for three different types of knowledge graphs which we call RDF-based graphs, property graphs and wikibase graphs. Although Shape Expressions were initially created to describe and validate RDF-based graphs, we present an extension of the language that can also be used to describe property graphs and wikibase graphs. An important problem of knowledge graphs is the large amount of data which jeopardizes their practical application. In order to palliate the problem, one approach is to create subsets of those knowledge graphs for some domains. We review some approaches that can be used to generate those subsets employing descriptions of the subsets using the Shape Expressions language.

3.2 Introduction

Review all the introduction. Empezar con alguna frase chula sobre grafos de conocimiento...

Since Google announced in 2012 the use of knowledge graphs to improve their search results in 2012 [64], Knowledge Graphs have been increasingly adopted by the industry. Several companies like Airbnb [10], Amazon [35], eBay [57], Facebook [53], IBM [16], LinkedIn [26], Microsoft [63], Uber [25], etc. have already announced their use of some kind of Knowledge Graphs.

Hablar de los 3 tipos de grafos de conocimiento tratados en el paper brevemente

There have been several approaches to represent knowledge using graphs. In this paper we will review and formalize three of them: RDF-based graphs, property graphs and wikibase graphs.

RDF-based graphs is one of the most well-known approaches given that RDF was proposed as a W3C recommendation already in 1999 [54] and a large ecosystem of tools have been created around it. An important aspect of RDF is the use of URIs, which facilitates interoperability.

re a bit about
data? SPARQL?

On the other hand, graph databases like Neo4J have also been employed to represent knowledge graphs. They employ a data model which allows to annotate both vertices and edges with pairs of property-values and has become to be known as property graphs.

Wikidata started in 2012 as a support project for Wikipedia but has been evolving and acquiring more and more importance as a hub of public knowledge. The data model employed by Wikidata combined several aspects from RDF following linked data principles and from property graphs, allowing the annotation of statements by property-values using qualifiers and references. The software suite that implements Wikidata is known as Wikibase and can be used to represent other knowledge graphs with the same data model, we will refer to these kind of knowledge graphs as wikibase graphs.

algunas estadís-

Given that knowledge graphs usually capture information about some real world entities, it is common that their size increases with their usage. A good example is the evolution of Wikidata...

Motivation:

- Talk about why the success of knowledge graphs can also be a problem for performance...
- Talk about the success of ShEx as an intuitive language

once the paper
ed

The main contributions of this paper are:

- We created a formal model for Wikibase graphs
- We extended the ShEx language to describe Wikibase graphs
- We propose a common framework that facilitates the comparison between 3 types of knowledge graphs: RDF-based knowledge graphs, property graphs and wikibase graphs.
- We formalize several approaches to generate subsets of Wikibase graphs:
 - Item and property generated subgraphs
 - Matching-generation subgraphs
 - ShEx + Slurping
 - ShEx based traversal
 - ...

The structure of the paper is as follows: Section 3.3 presents some preliminary definitions about sets and graphs. Section 3.4 introduces knowledge graphs and presents 3 main types of knowledge graphs: RDF-based, Property graphs and Wikibase graphs. Section 3.5 presents techniques to describe knowledge graphs. We describe the Shape Expressions language that has been developed to describe RDF-based graphs, and we extend it to describe property graphs and wikibase graphs. Section 3.6 presents the problem of creating subsets of knowledge graphs and describes several approaches to create subsets of wikibase graphs. Section 3.7 describes some real-world applications where it is important to generate subsets of knowledge graphs. Section 3.8 presents some results of those applications. Finally, section 3.9 reviews the related work and section 3.10 presents some

conclusions.

3.3 Preliminaries

Definitions

In this section, we provide some basic definitions that we will use in the rest of the paper.

Sets

. The finite set with elements a_1, \dots, a_n is written $\{a_1, \dots, a_n\}$, \emptyset represents the empty set, $S_1 \cup S_2$ is the union of sets S_1 and S_2 , $S_1 \cap S_2$ the intersection and $S_1 \times S_2$ the Cartesian product. $\text{FinSet}(S)$ represents the set of all finite subsets of S . A tuple $\langle A_1, \dots, A_n \rangle$ is the cartesian product $A_1 \times \dots \times A_n$.

Given a set S , its set of partitions is defined as $\text{part}(s) = \{(s_1, s_2) \mid s_1 \cup s_2 = s \wedge s_1 \cap s_2 = \emptyset\}$.

Definition 3.3.1 — Graph. A *graph* is a tuple $G = \langle \mathcal{V}, \mathcal{E} \rangle$, where \mathcal{V} is a set of nodes, and $\mathcal{E} \subseteq \mathcal{V} \times \mathcal{E} \times \mathcal{V}$ is a set of edges.

A multigraph is a graph where it is possible to have more than one edge between the same two nodes.

Definition 3.3.2 — Directed edge-labelled graph. A *directed edge-labelled graph* is a tuple $\mathcal{G} = \langle \mathcal{V}, \mathcal{E}, \mathcal{P} \rangle$, where \mathcal{V} is a set of nodes, \mathcal{P} is a set of labels also called predicates or properties, and $\mathcal{E} \subseteq \mathcal{V} \times \mathcal{L} \times \mathcal{V}$ is a set of edges. Each element $(x, p, y) \in \mathcal{E}$ is called a triple, where x is the subject, p is the predicate or property and y is the object.

Definition 3.3.3 — Triple-based graphs. A *triple-based graphs* is a directed edge-labelled graph $\mathcal{G} = \langle \mathcal{S}, \mathcal{P}, \mathcal{O}, \rho \rangle$ where \mathcal{S} is a set of subjects, \mathcal{P} is a set of predicates or properties and \mathcal{O} is a set of objects or values, and $\rho \subseteq \mathcal{S} \times \mathcal{P} \times \mathcal{O}$. Those sets don't need to be disjoint, and usually $\mathcal{P} \subseteq \mathcal{S} \subseteq \mathcal{O}$.

Definition 3.3.4 — Hypergraph. A *hypergraph* is a tuple $G = \langle \mathcal{V}, \mathcal{E} \rangle$ where \mathcal{V} is a set of nodes and $\mathcal{E} \subseteq \text{FinSet}(\mathcal{V})$ is a set of edges. Notice that \mathcal{E} is a family of subsets of vertices.

Definition 3.3.5 — Shape assignment. Given a graph \mathcal{G} with vertex set \mathcal{V} and a finite set of labels \mathcal{L} , a *shape assignment* over \mathcal{G} and \mathcal{L} is a subset of $\mathcal{V} \times \mathcal{L}$. We use τ to denote shape assignments, and we write $n@l$ instead of (n, l) for elements of shape assignments. Note that shape assignments correspond to shape maps in [59] and typings in [5, 65].

Bag

Regular bag exp

Regular bag exp
matching

3.4 Knowledge graphs models

Although the term *knowledge graphs* was already in use in the 1970s [60], the current notion of knowledge graphs was popularized by Google in 2012 [64].

We adopt an informal definition of knowledge graphs which has been inspired by Hogan et al [29]:

Definition 3.4.1 — Knowledge graph. A *Knowledge graph* is graph of data intended to represent knowledge of some real world domain, whose nodes represent entities of interest and whose edges represent relations between these entities.

review

The previous definition is deliberately open. The main feature of a knowledge graph is that it is intended to represent information about entities of some real world domain using a graph-based data structure.

Knowledge graphs are usually classified as:

- **Licence/proprietor:** There are public and open knowledge graphs like Yago [66], DBpedia [39] or Wikidata [70] as well as enterprise-based and proprietary knowledge graphs [53] like Google, Amazon, etc.
- **Scope:** there are general-purpose knowledge graphs which contain information about almost all domains like Wikidata as well as domain specific knowledge graphs which contain information from some specific domains like healthcare, education, chemistry, biology, cybersecurity, etc. [1]

Knowledge graphs can be represented using multiple technologies and in fact, the information about how Google's knowledge graph is implemented is not public. Nevertheless, in this paper, we will focus on three main technologies:

- **RDF based knowledge graphs** represent information using directed graphs whose edges are labels.
- **Property graphs** allow property–value pairs and a label to be associated with nodes and edges. Property graphs have been implemented by several popular graph databases like Neo4j [3].
- **Attributed graphs** allow property-value pairs associated with edges to add meta-data about the relationship represented by the edge and the values of those properties can themselves be nodes in the graph. The main example in this category is Wikidata where property-value pairs encode qualifiers and references.

3.4.1 RDF based knowledge graphs

Resource Description Framework (RDF) [14], is a W3C recommendation which is based on directed edge-labelled graphs.

The RDF data model defines different types of nodes, including *Internationalized Resource Identifiers (IRIs)* [17] which can be used to globally identify entities on the Web; literals, which allow for representing strings (with or without language tags) and values from other datatypes (integers, decimals, dates, etc.); and *blank nodes*. Blank nodes can be considered as existential variables that denote the existence of some resource for which an IRI or literal is not known or provided. They are locally scoped to the file or RDF store, and are not persistent or have portable identifiers [28].

Definition 3.4.2 — RDF Graph. Given a set of IRIs \mathcal{I} , a set of blank nodes \mathcal{B} and a set of literals \mathcal{Lit} , an *RDF graph* is a triple based graph $\mathcal{G} = \langle \mathcal{S}, \mathcal{P}, \mathcal{O}, \rho \rangle$ where $\mathcal{S} = \mathcal{I} \cup \mathcal{B}$, $\mathcal{P} = \mathcal{I}$, $\mathcal{O} = \mathcal{I} \cup \mathcal{B} \cup \mathcal{Lit}$ and $\rho \subseteq \mathcal{S} \times \mathcal{P} \times \mathcal{O}$

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

■ **Example 3.1** As a running example, we will represent information about Tim Berners-Lee declaring that he was born in London, on 1955, and was employed by CERN and London's country is UK. That information can be encoded in Turtle as:

```
prefix :      <http://example.org/>
prefix xsd:   <http://www.w3.org/2001/XMLSchema#>

:timbl      :birthPlace      :London ;
            :birthDate       "1955-08-06"^^xsd:date ;
            :employer        :CERN .
:London     :country         :UK .
```

Review the visualization after removing foundingMember information and added awards

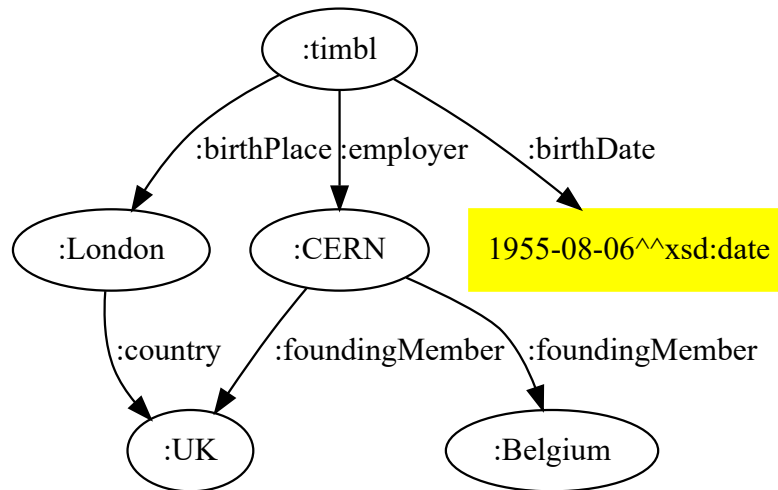


Figure 3.1: Example graph representation of RDF data

Figure 3.1 shows a possible visualization of that RDF graph using RDFShape, a tool developed by the authors of this paper which allows to play with RDF graphs¹ [36]:

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

RDF can be considered the basic element of the semantic web technology stack, forming a simple knowledge representation language on top of which several technologies have been developed like SPARQL for querying RDF data as well as RDFS and OWL to describe vocabularies and ontologies.

RDF reification and RDF-*

An important aspect of RDF as a knowledge representation formalism is to be able to represent information about RDF triples themselves, which is called reification. In this section we will present some of the possible approaches for reification using a simple example to help understand the approach used by Wikibase to serialize its data model to RDF. We also present the RDF-* approach which has become popular in the RDF-ecosystem with its support by several RDF stores like GraphDB².

■ **Example 3.2** As an example, we may want to qualify the statement that Tim Berners-Lee was employed by CERN, declaring that he was employed at two different points in time: in 1980 and between 1984 and 1994.

Several approaches have already been proposed RDF reification [27]:

- Standard RDF reification was introduced in RDF 1.0 [44]. It consists of using the predicates `rdf:subject`, `rdf:predicate` and `rdf:object` as well as the class `rdf:Statement` to explicitly declare statements.

```

_:s1 rdf:type      rdf:Statement ;
     rdf:subject   :timbl ;
     rdf:predicate :employer ;
     rdf:object    :CERN ;
     :start        "1980"^^xsd:gYear ;
     :end          "1980"^^xsd:gYear .
  
```

¹It is possible to interactively play with the example following this permalink: <https://rdfshape.weso.es/link/16275427216>

²<https://www.ontotext.com/knowledgehub/fundamentals/what-is-rdf-star/>

```
_:s2 rdf:type          rdf:Statement ;
    rdf:subject        :timbl ;
    rdf:predicate      :employer ;
    rdf:object         :CERN ;
    :start              "1984"^^xsd:gYear ;
    :end                "1994"^^xsd:gYear .
```

- Create a statement that models the n-ary relation [18]. For example, we can create two nodes :s1 and :s2 to represent the the 2 employments of Tim-Berners-Lee at CERN.

```
:timbl :employer :s1, :s2.
:s1 :employerV :CERN;
    :start      "1980"^^xsd:gYear ;
    :end        "1980"^^xsd:gYear .
:s2 :employerV :CERN;
    :start      "1984"^^xsd:gYear ;
    :end        "1994"^^xsd:gYear .
```

- Create *singleton properties* for each statement and link those properties with a specific predicate to the real property [51].

```
:timbl :employer1 :CERN ;
       :employer2 :CERN .

:employer1 :singletonPropertyOf :employer ;
    :start "1980"^^xsd:date ;
    :end   "1980"^^xsd:date .

:employer2 :singletonPropertyOf :employer ;
    :start "1984"^^xsd:date ;
    :end   "1994"^^xsd:date .
```

- RDF1.1 [14] included the concept of named graphs, which can be used to associate each triple with a different graph.

```
:g1 :timbl :employer :CERN .
:g1 :employed :start "1980"^^xsd:date .
:g1 :employed :end   "1980"^^xsd:date .
:g2 :timbl :employer :CERN .
:g2 :employed :start "1984"^^xsd:date .
:g2 :employed :end   "1994"^^xsd:date .
```

- RDF-* [15] has been recently introduced as an extension of RDF that includes RDF graphs as either the subjects or objects of a statement.

```
<<:timbl :employer :CERN>> :start "1980"^^xsd:gYear ;
                             :end   "1980"^^xsd:gYear .
<<:timbl :employer :CERN>> :start "1984"^^xsd:gYear ;
                             :end   "1994"^^xsd:gYear .
```

- Wikidata's RDF serialization follows a hybrid approach using a direct link to capture the preferred value and singleton nodes that represent the statements capturing the n-ary relationship [18]. It also follows a convention that employs the same local name of the property preceded by different namespaces: wdt: for the direct link, p for the link between the node and the singleton statements, ps: for the link between the singleton statements and the values, and pq: for the link between the singleton statements and the qualified values. The previous

example using Wikidata RDF serialization could be ³:

```
:timbl wdt:employer :CERN .
:timbl p:employer :s1 .
:timbl p:employer :s2 .
:s1 ps:employer :CERN ;
pq:start "1980"^^xsd:gYear ;
pq:end "1980"^^xsd:gYear .
:s2 ps:employer :CERN ;
pq:start "1984"^^xsd:gYear ;
pq:end "1994"^^xsd:gYear .
```

■

3.4.2 Property graphs

Property graphs have become popular thanks to several commercial graph databases like Neo4j ⁴, JanusGraph ⁵ or Sparksee ⁶. 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 [62].

Definition 3.4.3 — Property graph. Given a set of types \mathcal{T} , a set of properties \mathcal{P} , and a set of values \mathcal{V} , a *property graph* \mathcal{G} is a tuple $\langle \mathcal{N}, \mathcal{E}, \rho, \lambda_n, \lambda_e, \sigma \rangle$ where $\mathcal{N} \cap \mathcal{E} = \emptyset$, $\rho : \mathcal{E} \mapsto \mathcal{N} \times \mathcal{N}$ is a total function, $\lambda_n : \mathcal{N} \mapsto \text{FinSet}(\mathcal{T})$, $\lambda_e : \mathcal{E} \mapsto \mathcal{T}$, and $\sigma : \mathcal{N} \cup \mathcal{E} \times \mathcal{P} \mapsto \text{FinSet}(\mathcal{V})$.

A property graph is formed by a set of node identifiers \mathcal{N} and a set of edges \mathcal{E} where ρ associates a pair of nodes (n_1, n_2) to every $e \in \mathcal{E}$ 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 $i \in \mathcal{N} \cup \mathcal{E}$ is a node or edge and $p \in \mathcal{P}$ is a property.

■ **Example 3.3** As an example, we will represent information about Tim Berners-Lee in a property graph encoding his birth place with a relation to a node that represents London, and his birth date with a value for that property in the same node. We can also represent that its employer has been CERN in two times, one in 1980, and another between 1984 and 1994.

$\mathcal{T} = \{\text{Human}, \text{City}, \text{Metropolis}, \text{Country}, \text{Organization}, \text{birthPlace}, \text{country}, \text{employer}\}$

$\mathcal{P} = \{\text{label}, \text{birthDate}, \text{start}, \text{end}\}$

$\mathcal{V} = \{\text{Tim Berners-Lee}, 1955, 1980, 1984, 1994, \text{London}, \text{UK}\}$

$\mathcal{N} = \{n_1, n_2, n_3, n_4\} \quad \mathcal{E} = \{r_1, r_2, r_3, r_4\}$

$\rho = r_1 \mapsto (n_1, n_2), r_2 \mapsto (n_2, n_3), r_3 \mapsto (n_1, n_4), r_4 \mapsto (n_1, n_4)$

$\lambda_n = n_1 \mapsto \{\text{Human}\}, n_2 \mapsto \{\text{City}, \text{Metropolis}\}, n_3 \mapsto \{\text{Country}\}, n_4 \mapsto \{\text{Organization}\}$

$\lambda_e = r_1 \mapsto \text{birthPlace}, r_2 \mapsto \text{country}, r_3 \mapsto \text{employer}, r_4 \mapsto \text{employer}$

$\sigma = (n_1, \text{label}) \mapsto \text{Tim Berners-Lee}, (n_1, \text{birthDate}) \mapsto 1955$

$(n_2, \text{label}) \mapsto \text{London}, (n_3, \text{label}) \mapsto \text{UK}, (n_4, \text{label}) \mapsto \text{CERN}$

$(r_3, \text{start}) \mapsto 1980, (r_3, \text{end}) \mapsto 1980, (r_4, \text{start}) \mapsto 1984, (r_4, \text{end}) \mapsto 1994$

■

³We omit the representation of values and use English names instead of numbers for clarity

⁴<https://neo4j.com/>

⁵<https://janusgraph.org/>

⁶<https://www.sparsity-technologies.com/#sparksee>

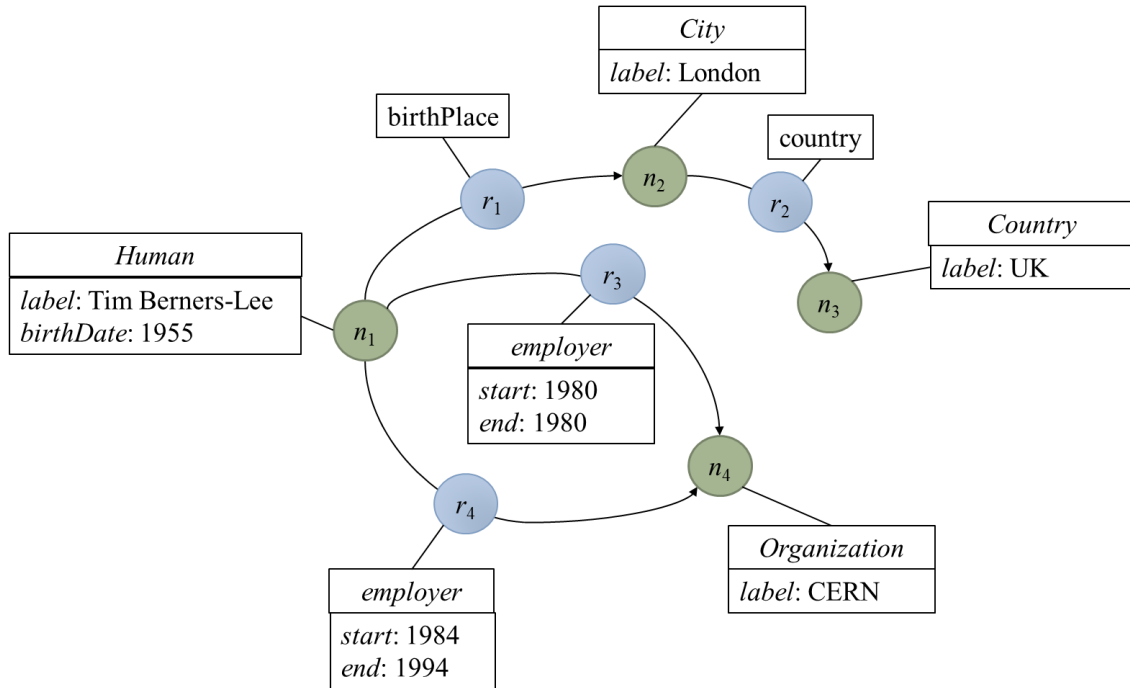


Figure 3.2: Example graph visualization of a property graph

Figure 3.2 presents a possible visualization of a property graph.

Review the figure to remove long dates and add metropolis

Cypher is a property graph query language that was initially developed for Neo4j [20]. The following Cypher script can generate the property graph represented in figure 3.2:

```
CREATE (n1:Human {label:'Tim Berners-Lee', birthDate:1955})
CREATE (n2:City:Metropolis {label:'London'})
CREATE (n3:Country {label:'UK'})
CREATE (n4:Organization {label:'CERN'})
CREATE
  (n1)-[:birthPlace]->(n2),
  (n2)-[:country]->(n3),
  (n1)-[:employer {start:[1980], end:[1980]}]->(n4),
  (n1)-[:employer {start:[1984], end:[1994]}]->(n4),
```

As can be seen in previous example, property graphs are multigraphs because it is possible to have more than one edges between nodes.

3.4.3 Wikibase graphs

Wikidata⁷ started in 2012 to support Wikipedia [70]. It has become one of the biggest human knowledge bases, maintained both by humans collaboratively as by bots, which update the contents from external services or databases. Several organizations are donating their data to Wikidata and collaborate in its maintenance providing resources. A remarkable case is Google, which migrated its previous knowledge graph Freebase to Wikidata in 2017 [67].

Apart of Wikipedia, Wikidata has been reported to be used by external applications like Apple's Siri⁸ and it has been adopted as the central hub for knowledge in several domains like life

⁷<http://wikidata.org/>

⁸<https://lists.wikimedia.org/pipermail/wikidata/2017-July/010919.html>

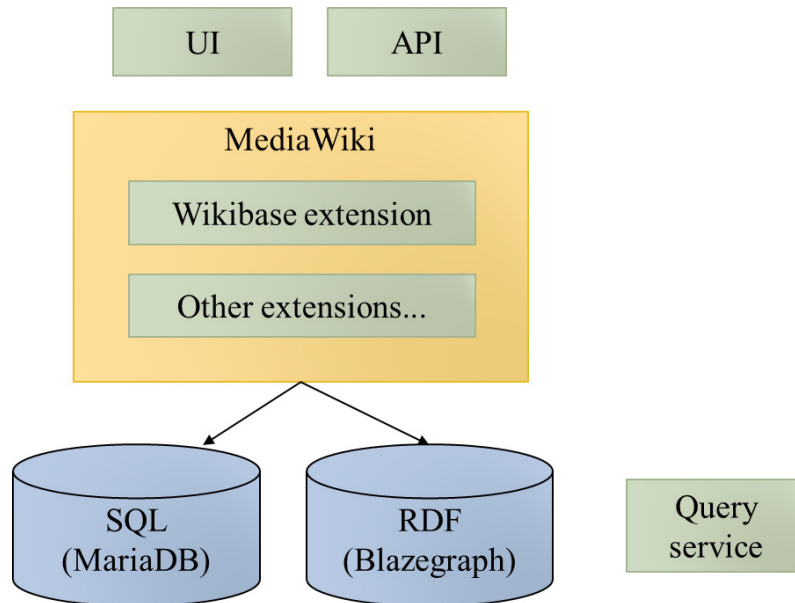


Figure 3.3: Simplified architecture of Wikibase

sciences [8], libraries [61] or social science [13]. As of August, 2021, it contains information about more than 94 millions of entities ⁹ and since its launch there have been more than 1,400 millions of edits.

Wikibase ¹⁰ is a set of open source tools which run Wikidata. With Wikibase it is possible to create Knowledge graphs that follow the same data model as Wikidata but that represent information from other domains. The projects that are using Wikibase are called Wikibase instances, some examples of wikibase instances are Rhizome ¹¹ or Enslaved ¹². Given that Wikidata was the first and most common Wikibase instance the terms are sometimes used indistinctly.

Wikibase was initially created from MediaWiki software which ensured adoption by the Wikimedia community. Internally, Wikidata content is managed by a relational database (MariaDB) which consists of strings stored and versioned as character blobs [43]. but was not suitable for advanced data analysis and querying. With the goal of facilitating those tasks and integrate Wikibase within the semantic web ecosystem, the Wikimedia Foundation adopted Blazegraph ¹³ as a complementary triplestore and graph database. In this way, there are 2 main data models that coexist in Wikibase: a document-centric model based on MediaWiki and an RDF-based model based on RDF which can be used to do SPARQL queries through the Query Service.

A simplified view of Wikibase architecture is depicted in figure 3.3 ¹⁴.

Wikibase data model: informal introduction

The Wikibase data model ¹⁵ is defined as an abstract data model that can have different serializations like JSON and RDF. It is defined using UML data structures and a notation called Wikidata Object Notation.

⁹<https://www.wikidata.org/wiki/Wikidata:Statistics>

¹⁰<https://wikiba.se/>

¹¹<https://rhizome.org/about/>

¹²<https://enslaved.org/>

¹³<https://blazegraph.com/>

¹⁴A more in-depth view of Wikibase architecture can be found at <https://addshore.com/2018/12/wikidata-architecture-overview-diagrams/>

¹⁵<https://www.mediawiki.org/wiki/Wikibase/DataModel>

Informally, the Wikibase data model is formed from entities and statements about those entities. An entity can either be an item or a property. An item is usually represented using a Q followed by a number and can represent any thing like an abstract or concrete concept. For example, Q80 represents Tim Berners-Lee in Wikidata.

A property is usually represented by a P followed by a number and represents a relationship between an item and a value. For example, P19 represents the property *place of birth* in Wikidata.

The values that can be associated to a property are constrained to belong to some specific datatype. There can be compound datatypes like geographical coordinates.

The current list of datatypes are: quantities, dates and times, geographic locations, geographic shapes, web resources, items, properties, media, non-translated strings, monolingual and multilingual texts/multitexts.

A statement consists of:

- A property which is usually denoted using a P followed by a number.
- A declaration about the possible value (in wikibase terms, it is called a *snak*) which can be a specific value, no value declaration or a some value declaration.
- A rank declaration which can be either preferred, normal or deprecated.
- Zero or more qualifiers which consist of a list of property-value pairs
- Zero or more references which consist of a list of property-value pairs.

Wikibase data model: formal definition

We define a formal model for Wikibase which is based on Multi-Attributed Relational Structures (MARS) [50]. For brevity, we model both qualifiers and references as attributes and don't handle the no-value and some-value snaks.

Definition 3.4.4 — Wikibase graphs. Given a mutually disjoint set of items \mathcal{Q} , a set of properties \mathcal{P} and a set of data values \mathcal{D} , a *Wikibase graph* is a tuple $\langle \mathcal{Q}, \mathcal{P}, \mathcal{D}, \rho \rangle$ such that $\rho \subseteq \mathcal{E} \times \mathcal{P} \times \mathcal{V} \times \text{FinSet}(\mathcal{P} \times \mathcal{V})$ where $\mathcal{E} = \mathcal{Q} \cup \mathcal{P}$ is the set of entities which can be subjects of a statement and $\mathcal{V} = \mathcal{E} \cup \mathcal{D}$ is the set of possible values of a property.

In practice, Wikibase graphs also add the constraint that every item $q \in \mathcal{Q}$ (or property $p \in \mathcal{P}$) has a unique integer identifier $q^i \in \mathbb{N}$ ($p^i \in \mathbb{N}$).

In the Wikibase data model, statements contain a list of properties-values and the values can themselves be nodes from the graph. This is different from property graphs, where the set of vertices and the set of values are disjoint.

■ **Example 3.4 — Running example as a Wikibase graph.** We continue with the running example about Tim Berners-lee, but extend it with more information about awards. More concretely, we add the information that Tim Berners-Lee was awarded with the *Princess of Asturias* (PA) award together with Vinton Cerf (vintCerf)¹⁶, and that the country of that award is Spain:

¹⁶The award was really obtained by Tim Berners-Lee, Vinton Cerf, Robert Kahn and Lawrence Roberts, we included here only the first two for simplicity

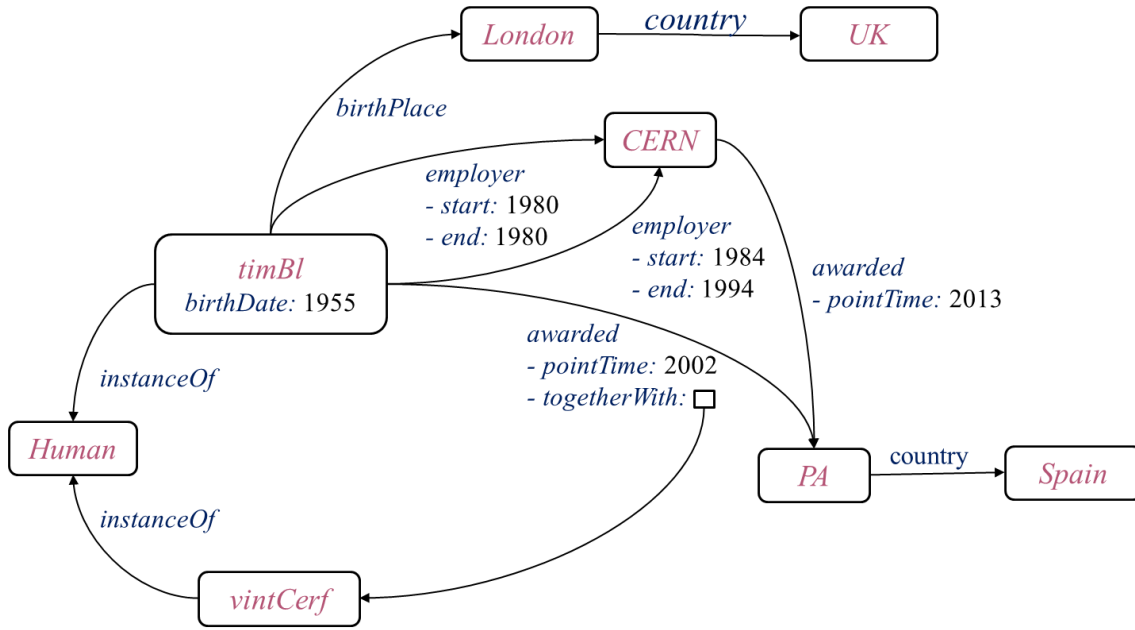


Figure 3.4: Visualization of example wikibase graph

$\mathcal{Q} = \{ \text{timBl, vintCerf, London, CERN, UK, Spain, PA, Human} \}$
 $\mathcal{P} = \{ \text{birthDate, birthPlace, country, employer, awarded, start, end, pointTime, togetherWith, instanceOf} \}$
 $\mathcal{D} = \{ 1984, 1994, 1980, 1955 \}$
 $\rho = \{ (\text{timBl, instanceOf, Human, } \{\}),$
 $(\text{timBl, birthDate, 1955, } \{\}),$
 $(\text{timBl, birthPlace, London, } \{\}),$
 $(\text{timBl, employer, CERN, } \{ \text{start:1980, end:1980} \}),$
 $(\text{timBl, employer, CERN, } \{ \text{start:1984, end:1994} \}),$
 $(\text{timBl, awarded, PA, } \{ \text{pointTime: 2002, togetherWith: vintCerf} \}),$
 $(\text{London, country, UK, } \{\}),$
 $(\text{vintCerf, instanceOf, Human, } \{\})$
 $(\text{CERN, awarded, PA, } \{ \text{pointTime: 2013} \})$
 $(\text{PA, country, Spain, } \{\}) \}$

Figure 3.4 presents a possible visualization of a wikibase graph. ■

The Wikibase data model supports 2 main export formats: JSON and RDF. The JSON one directly follows the structure of the Wikibase data model and is employed by the JSON Dumps while the RDF serialization follows semantic web and linked data principles.

Wikibase JSON serialization

The JSON serialization follows the Wikibase data model. It basically consists of an array of entities where each entity is a JSON object that captures all the local information about the entity: the labels, descriptions, aliases, sitelinks and statements that have the entity as subject. Each JSON object is represented in a single line. A remarkable feature of this encoding is that it captures the output neighbourhood of every entity in a single line making it amenable to processing models that

focus on local neighbourhoods because the whole graph can be processed in a single pass.

```
[
  { "type": "item", "id": "Q42", "claims": { "P31": [...
  { "type": "item", "id": "Q80", "claims": { "P108": [...
  { "type": "property", "id": "P108", "claims": { ...
  ...
]
```

Wikibase RDF serialization

The RDF serialization¹⁷ of Wikidata was designed with the goal of being able to represent all the structures of the Wikibase data model in RDF, maintaining compatibility with semantic web vocabularies like RDFS and OWL and avoiding the use of blank nodes [18].

■ **Example 3.5 — RDF serialization of a node.** As an example, the information about Tim Berners-Lee (Q80) declaring that he was as employer (P108) of CERN (Q42944) between 1984 and 1994 is represented as ¹⁸:

```
wd:Q80 rdf:type wikibase:Item ;
  wdt:P108 wd:Q42944 ;
  p:P108 :Q80-4fe7940f .

:Q80-4fe7940f rdf:type wikibase:Statement ;
  wikibase:rank wikibase:NormalRank ;
  ps:P108 wd:Q42944 ;
  pq:P580 "1984-01-01T00:00:00Z"^^xsd:dateTime ;
  pq:P582 "1994-01-01T00:00:00Z"^^xsd:dateTime .
```

The RDF serialization uses a direct arc to represent the preferred statement represented by prefix alias `wdt`: leaving the rest of the values of a property accessible through the namespaces `p:`, `ps:` and `pq:`.

The reification model employed by Wikidata creates auxiliary nodes that represent each statement. In the previous example, the node `:Q80-4fe7940f` represents the statement which can be qualified with the start and end time.

■

Apart of the the dumps, RDF serialization is also employed by the Wikidata Query Service [4, 42] and users of Wikidata are required to use and understand the singleton statement approach and namespace conventions employed.

Add an example SPARQL query to obtain Tim Berners-Lee employers and start-end dates

We could define how we can convert Wikibase graphs to RDF graphs

¹⁷https://www.mediawiki.org/wiki/Wikibase/Indexing/RDF_Dump_Format

¹⁸The full Turtle serialization can be obtained at: <https://www.wikidata.org/wiki/Special:EntityData/Q80.ttl>

3.5 Describing Knowledge Graphs

3.5.1 Describing and validating RDF

At the end of 2013, an *RDF Validation Workshop*¹⁹ was organized by W3C/MIT to discuss use cases and requirements related with the quality of RDF data. One of the conclusions of the workshop was that there was a need for a high-level language that could describe and validate RDF data.

Shape Expressions (ShEx) were proposed as such a language in 2014 [58]. It was designed as a high-level and concise domain-specific language to describe RDF. The syntax of ShEx is inspired by Turtle and SPARQL, while the semantics is inspired by RelaxNG and XML Schema.

In this section we describe a simplified abstract syntax of ShEx following [6]²⁰.

Definition 3.5.1 — ShEx schema. A *ShEx Schema* is defined as a tuple $\langle \mathcal{L}, \delta \rangle$ where \mathcal{L} set of shape labels, and $\delta : \mathcal{L} \rightarrow \mathcal{S}$ is a total function from labels to shape expressions.

The set of shape expressions $se \in \mathcal{S}$ is defined using the following abstract syntax:

se	$::=$	$cond$	Basic boolean condition on nodes (node constraint)
		$ $	s Shape
		$ $	$se_1 \text{ AND } se_2$ Conjunction
		$ $	$@l$ Shape label reference for $l \in \mathcal{L}$
s	$::=$	$CLOSED \{te\}$	Closed shape
		$ $	$\{te\}$ Open shape
te	$::=$	$te_1;te_2$	Each of te_1 and te_2
		$ $	$te_1 te_2$ Some of te_1 or te_2
		$ $	te^* Zero or more te
		$ $	ϵ Empty triple expression
		$ $	$\neg \xrightarrow{p} @l$ Triple constraint with predicate p

Intuitively, shape expressions define conditions about nodes while triple expressions define conditions about the neighborhood of nodes, and shapes qualify those neighborhoods by disallowing triples with other predicates in the case of closed shapes or allowing them in the case of open shapes.

In this paper we omit the negation and disjunction operator to facilitate the presentation of the subsetting semantics. Adding those operators increases the expressiveness of ShEx to validate RDF graphs but we consider that their use to create subsets is not yet clear so we leave them for further research.

The restrictions imposed on shape expressions schemas in [59] also apply here. Namely, in a schema $(\mathcal{L}, \delta, \mathcal{S})$

- 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 \mathcal{L} ;
- no definition $\delta(l)$ uses a reference $@l$ to itself, neither directly nor transitively, except while traversing a shape. For instance, $\delta(l) = @l \text{ AND } se$ is forbidden, but $\delta(l) = \{ \neg \xrightarrow{p} @l \}$ is allowed.

■ **Example 3.6 — Example of ShEx schema.** A ShEx schema that describes the RDF graph presented in example 3.1 can be defined as:

¹⁹<https://www.w3.org/2012/12/rdf-val/>

²⁰The full specification of ShEx is available at <https://shex.io/shex-semantics/>

$$\begin{aligned}
\mathcal{L} &= \{ \text{Person, Place, Country, Organization, Date} \} \\
\delta(\text{Person}) &= \{ \text{ } \xrightarrow{\text{birthDate}} \text{ @Date; } \xrightarrow{\text{birthPlace}} \text{ @Place; } \\
&\quad \xrightarrow{\text{employer}} \text{ @Organization* } \} \\
\delta(\text{Place}) &= \{ \text{ } \xrightarrow{\text{country}} \text{ @Country} \} \\
\delta(\text{Country}) &= \{ \text{ } \} \\
\delta(\text{Organization}) &= \{ \text{ } \} \\
\delta(\text{Date}) &= \text{ xsd:Date}
\end{aligned}$$

ShEx has several concrete syntaxes like a compact syntax (ShExC) and an RDF syntax defined based on JSON-LD (ShExJ) ²¹.

■ **Example 3.7 — Example of ShEx in ShExC compact syntax.** The previous ShEx schema can be defined using the compact syntax as:

```

:Person {
  :birthPlace @:Place ;
  :birthDate @:Date ;
  :employer @:Organization ;
}
:Place {
  :country @:Country
}
:Country {}
:Organization {}
:Date {}

```

when rdfshape again...

In general, it is possible to visualize ShEx schemas using UML-like class diagrams. Figure 3.5 presents a visualization of the previous schema using RDFShape ²²

Apart of describing RDF data, Shape Expressions have been designed to enable validation and checking if an RDF node conforms to some shape.

The semantics of Shape Expression validation can be defined with a relation between an RDF node, an RDF graph, a ShEx schema and a shape assignment.

As an example of validation, we have implemented the ShEx-s library which is used by RDFShape ²³.

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

The following rules are defined similar [5], where it is shown that there exists a unique maximal shape assignment τ_{\max} that allows to define conformance independently on the shape assignment.

The conformance relation is defined recursively on the structure of se by the set of inference rules presented below.

the change of open shape

the order of ce rules...

²¹ See [59] for details.

²² This visualization can be interactively generated following: <https://rdfshape.weso.es/link/16275431752>

²³ It is possible to see the results of validating the previous example in RDFShape following this link: <https://rdfshape.weso.es/link/16275436158>

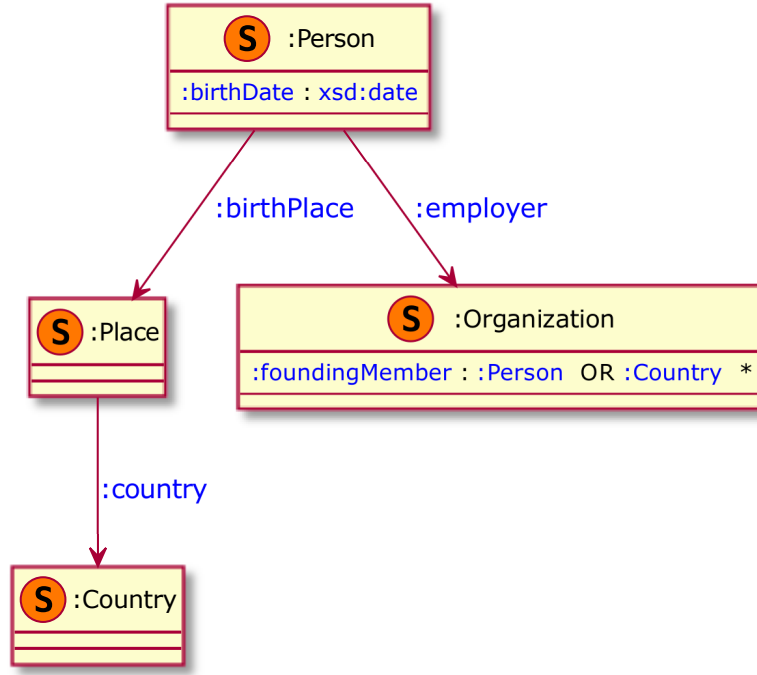
Generated by [rdfshape](#)

Figure 3.5: ShEx schema visualization as UML-like diagrams

$$\begin{array}{l}
 \text{Cond} \frac{\text{cond}(n) = \text{true}}{\mathcal{G}, n, \tau \models \text{cond}} \quad \text{AND} \frac{\mathcal{G}, n, \tau \models se_1 \quad \mathcal{G}, n, \tau \models se_2}{\mathcal{G}, n, \tau \models se_1 \text{ AND } se_2} \\
 \text{OR}_1 \frac{\mathcal{G}, n, \tau \models se_1}{\mathcal{G}, n, \tau \models se_1 \text{ OR } se_2} \quad \text{OR}_2 \frac{\mathcal{G}, n, \tau \models se_2}{\mathcal{G}, n, \tau \models se_1 \text{ OR } se_2} \\
 \text{NOT} \frac{\mathcal{G}, n, \tau \not\models se}{\mathcal{G}, n, \tau \models \text{NOT } se} \quad \text{ClosedShape} \frac{\text{neighs}(n, \mathcal{G}) = ts \quad \mathcal{G}, ts, \tau \models te}{\mathcal{G}, n, \tau \models \text{CLOSED } \{te\}} \\
 \text{OpenShape} \frac{ts = \{\langle x, p, y \rangle \in \text{neighs}(n, \mathcal{G}) \mid p \in \text{preds}(te)\} \quad \mathcal{G}, ts, \tau \models te}{\mathcal{G}, n, \tau \models \{te\}}
 \end{array}$$

where $\text{preds}(te)$ is the set of predicates that appear in a triple expression te and can be defined as:

$$\begin{array}{ll}
 \text{preds}(te_1; te_2) &= \text{preds}(te_1) \cup \text{preds}(te_2) \\
 \text{preds}(te_1 \mid te_2) &= \text{preds}(te_1) \cup \text{preds}(te_2) \\
 \text{preds}(\sqcup \xrightarrow{p} te) &= \{p\} \\
 \text{preds}(te^*) &= \text{preds}(te) \\
 \text{preds}(\epsilon) &= \emptyset
 \end{array}$$

The rules for node constraint (Cond), conjunction, disjunction, and negation, are as expected. A node n conforms to an open shape with triple expression te if its neighbourhood 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 neighbourhood of the node (rule ClosedShape).

Conformance to a shape uses a second conformance relation defined on sets on neighbourhood triples ts instead of nodes n . The set of neighbourhood nodes ts of a graph \mathcal{G} conforms to a triple expression te with shape assignment τ , written as $\mathcal{G}, ts, \tau \models te$, as defined by the following

inference rules recursively on the structure of te .

$$\begin{array}{c}
 \text{EachOf} \frac{(ts_1, ts_2) \in \text{part}(ts) \quad \mathcal{G}, ts_1, \tau \Vdash te_1 \quad \mathcal{G}, ts_2, \tau \Vdash te_2}{\mathcal{G}, ts, \tau \Vdash te_1; te_2} \\
 \\
 \text{OneOf}_1 \frac{\mathcal{G}, ts, \tau \Vdash te_1}{\mathcal{G}, ts, \tau \Vdash te_1 \mid te_2} \quad \text{OneOf}_2 \frac{\mathcal{G}, ts, \tau \Vdash te_2}{\mathcal{G}, ts, \tau \Vdash te_1 \mid te_2} \\
 \\
 \text{TripleConstraint} \frac{ts = \{\langle x, p, y \rangle\} \quad \mathcal{G}, y, \tau \models @l}{\mathcal{G}, ts, \tau \Vdash \xrightarrow{p} @l} \quad \text{Star}_1 \frac{}{\mathcal{G}, \emptyset, \tau \Vdash te^*} \\
 \\
 \text{Star}_2 \frac{(ts_1, ts_2) \in \text{part}(ts) \quad \mathcal{G}, ts_1, \tau \Vdash te \quad \mathcal{G}, ts_2, \tau \Vdash te^*}{\mathcal{G}, ts, \tau \Vdash te^*}
 \end{array}$$

We are now ready to define the semantics of ShEx schemas independently on shape assignments. A shape assignment τ for graph \mathcal{G} and \mathcal{S} is called *valid* if for every node n in \mathcal{G} and every shape expression label l defined in \mathcal{S} , if $n@l \in \tau$, then $\mathcal{G}, n, \tau \models @l$.

Lemma 3.5.1 — Boneva et al (6). For every graph \mathcal{G} , there exists a unique maximal valid shape assignment τ_{\max} such that if τ is a valid shape assignment for \mathcal{G} and \mathcal{S} , then $\tau \subseteq \tau_{\max}$.

out ShEx-*

3.5.2 Describing and validating Property graphs

In this section we define a ShEx extension called PShEx that can be used to describe and validate Property graphs. According to the definition of 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 that we will call qualifiers.

The language 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 and qualifier expressions (qs) that describe qualifiers sets of property/values associated with node/edge identifiers.

Definition 3.5.2 — PShEx schema. A *PShEx Schema* is a tuple $\langle \mathcal{L}, \delta \rangle$ where \mathcal{L} set of shape labels, and $\delta : \mathcal{L} \rightarrow \mathcal{S}$ is a total function from labels to shape expressions $se \in \mathcal{S}$ defined using the abstract syntax:

se	$::=$	$cond_{t_s}$	Basic boolean condition on set of types $t_s \subseteq \mathcal{T}$
		s	Shape
		$se_1 \text{ AND } se_2$	Conjunction
		$se_1 \text{ OR } se_2$	Disjunction
		$\text{NOT } se$	Negation
		$@l$	Shape label reference for $l \in \mathcal{L}$
		qs	Qualifiers of that node
s	$::=$	$\text{CLOSED } \{te\}$	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
		$\perp \xrightarrow{p} @l \text{ } qs$	Triple constraint with property type p whose nodes satisfy the shape l and qualifiers qs
qs	$::=$	$[ps]$	Open qualifier specifiers ps
		$\lceil ps \rceil$	Closed qualifier specifiers ps
ps	$::=$	ps_1, ps_2	Each of ps_1 and ps_2
		$ps_1 \mid ps_2$	OneOf of ps_1 or ps_2
		ps^*	zero of more ps
		$p : cond_v$	Property p with value conforming to $cond_v$ $cond_v$ is a boolean condition on sets of values $v_s \subseteq \mathcal{V}$

We will omit the list of qualifiers when it is empty.

■ **Example 3.8** As an example, we can define a PShEx schema that describes the property graph from example 3.3 where $hasType_t$ is a condition that is satisfied when the set of types of a node contains the type t , i.e. $hasType_t(vs) = \text{true}$ if $t \in vs$ and $String, Date$ are conditions on the values that are satisfied when the values have the corresponding type.

\mathcal{L}	$=$	$\{ \text{Person, Place, Country, Org} \}$
$\delta(\text{Person})$	$=$	$hasType_{\text{Human}} \text{ AND } [label : String, birthDate : Date] \text{ AND } \{$ $\quad \perp \xrightarrow{\text{birthPlace}} @Place;$ $\quad \perp \xrightarrow{\text{employer}} @Org [start : Date, end : Date]^*$ $\quad \}$
$\delta(\text{Place})$	$=$	$[label : String] \text{ AND } \{$ $\quad \perp \xrightarrow{\text{country}} @Country$ $\quad \}$
$\delta(\text{Country})$	$=$	$hasType_{\text{Country}} \text{ AND } [label : String] \{ \}$
$\delta(\text{Org})$	$=$	$hasType_{\text{Organization}} \text{ AND } [label : String] \{ \}$

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

■ **Definition 3.5.3 — Neighbourhood of node in property graph.** The neighbors of a node $n \in \mathcal{N}$ in a property graph $\mathcal{G} = \langle \mathcal{N}, \mathcal{E}, \rho, \lambda_n, \lambda_e, \sigma \rangle$ are defined as $neighs(n) = \{(n, p, y, vs) \mid \exists v \in \mathcal{E} \text{ such that } \rho(v) = (n, y) \wedge \lambda_e(v) = p \wedge vs = \{(k, v) \mid \sigma(k, v) = ws \wedge v \in ws\}\}$

■ **Example 3.9** The neighbors of node n_1 in property graph 3.3 are:

$neighs(n_1)$	$=$	$\{$
		$(n_1, \text{birthPlace}, n_2, \{ \}),$
		$(n_1, \text{employer}, n_4, \{(start, 1980), (end, 1980)\}),$
		$(n_1, \text{employer}, n_4, \{(start, 1984), (end, 1994)\}) \}$

The semantic specification of PShEx can be defined in a similar way to the ShEx one. Given

a property graph \mathcal{G} , and a shape assignment τ , a node identifier $n \in \mathcal{N}$ conforms with a shape expression se , which is represented as $\mathcal{G}, n, \tau \models se$ according to the following rules:

$$\begin{array}{c}
\text{Cond}_{ts} \frac{\lambda_n(n) = vs \quad \text{cond}_{ts}(vs) = \text{true}}{\mathcal{G}, n, \tau \models \text{cond}_{ts}} \quad \text{AND} \frac{\mathcal{G}, n, \tau \models se_1 \quad \mathcal{G}, n, \tau \models se_2}{\mathcal{G}, n, \tau \models se_1 \text{ AND } se_2} \\
\text{OR}_1 \frac{\mathcal{G}, n, \tau \models se_1}{\mathcal{G}, n, \tau \models se_1 \text{ OR } se_2} \quad \text{OR}_2 \frac{\mathcal{G}, n, \tau \models se_2}{\mathcal{G}, n, \tau \models se_1 \text{ OR } se_2} \\
\text{NOT} \frac{\mathcal{G}, n, \tau \not\models se}{\mathcal{G}, n, \tau \models \text{NOT } se} \quad \text{ClosedShape} \frac{\text{neighs}(n, \mathcal{G}) = ts \quad \mathcal{G}, ts, \tau \models s'}{\mathcal{G}, n, \tau \models \text{CLOSED } \{te\}} \\
\text{OpenShape} \frac{ts = \{\langle x, p, y \rangle \in \text{neighs}(n, \mathcal{G}) \mid p \in \text{preds}(te)\} \quad \mathcal{G}, ts, \tau \models te}{\mathcal{G}, n, \tau \models \{te\}}
\end{array}$$

where $\text{preds}(te)$ is the set of edge labels (or predicates) that appear in a triple expression te and can be defined as:

$$\begin{array}{ll}
\text{preds}(te_1; te_2) &= \text{preds}(te_1) \cup \text{preds}(te_2) \\
\text{preds}(te_1 \mid te_2) &= \text{preds}(te_1) \cup \text{preds}(te_2) \\
\text{preds}(_ \xrightarrow{p} te) &= \{p\} \\
\text{preds}(te^*) &= \text{preds}(te) \\
\text{preds}(\epsilon) &= \emptyset
\end{array}$$

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

$$\begin{array}{c}
\text{EachOf} \frac{(ts_1, ts_2) \in \text{part}(ts) \quad \mathcal{G}, ts_1, \tau \models te_1 \quad \mathcal{G}, ts_2, \tau \models te_2}{\mathcal{G}, ts, \tau \models te_1; te_2} \\
\text{OneOf}_1 \frac{\mathcal{G}, ts, \tau \models te_1}{\mathcal{G}, ts, \tau \models te_1 \mid te_2} \quad \text{OneOf}_2 \frac{\mathcal{G}, ts, \tau \models te_2}{\mathcal{G}, ts, \tau \models te_1 \mid te_2} \\
\text{TripleConstraint} \frac{ts = \{\langle x, p, y, s \rangle\} \quad \mathcal{G}, y, \tau \models @l \quad \mathcal{G}, s, \tau \models qs}{\mathcal{G}, ts, \tau \models _ \xrightarrow{p} @l qs} \\
\text{Star}_1 \frac{}{\mathcal{G}, \emptyset, \tau \models te^*} \\
\text{Star}_2 \frac{(ts_1, ts_2) \in \text{part}(ts) \quad \mathcal{G}, ts_1, \tau \models te \quad \mathcal{G}, ts_2, \tau \models te^*}{\mathcal{G}, ts, \tau \models te^*}
\end{array}$$

We declare a conformance relationship $\mathcal{G}, s, \tau \models qs$ between a graph \mathcal{G} a set $s \in P \times V$ of property-value elements, a shape assignment τ and a qualifier specifier qs .

$$\begin{array}{c}
\text{OpenQs} \frac{s' = \{(p, v) \in s \mid p \in \text{props}(ps)\} \quad \mathcal{G}, s', \tau \vdash ps}{\mathcal{G}, s, \tau \vdash \lfloor ps \rfloor} \quad \text{CloseQs} \frac{\mathcal{G}, s, \tau \vdash ps}{\mathcal{G}, s, \tau \vdash \lceil ps \rceil} \\
\\
\text{EachOfQs} \frac{\mathcal{G}, s, \tau \vdash ps_1 \quad \mathcal{G}, s, \tau \vdash ps_2}{\mathcal{G}, s, \tau \vdash ps_1, ps_2} \\
\\
\text{OneOfQs}_1 \frac{\mathcal{G}, s, \tau \vdash ps_1}{\mathcal{G}, s, \tau \vdash ps_1 \mid ps_2} \quad \text{OneOfQs}_2 \frac{\mathcal{G}, s, \tau \vdash ps_2}{\mathcal{G}, s, \tau \vdash ps_1 \mid ps_2} \\
\\
\text{StarQs}_1 \frac{}{\mathcal{G}, \emptyset, \tau \vdash ps^*} \quad \text{StarQs}_2 \frac{(s_1, s_2) \in \text{part}(s) \quad \mathcal{G}, s_1, \tau \vdash ps \quad \mathcal{G}, s_2, \tau \vdash ps^*}{\mathcal{G}, s, \tau \vdash ps^*} \\
\\
\text{PropertyQs} \frac{s = \{(p, w)\} \quad \text{conv}_v(w) = \text{true}}{\mathcal{G}, s, \tau \vdash p : \text{cond}_v}
\end{array}$$

where $\text{props}(ps)$ is the set of properties that appear in a property specifier ps and can be defined as:

$$\begin{aligned}
\text{props}(ps_1, ps_2) &= \text{props}(ps_1) \cup \text{props}(ps_2) \\
\text{props}(ps_1 \mid ps_2) &= \text{props}(ps_1) \cup \text{props}(ps_2) \\
\text{props}(ps^*) &= \text{preds}(ps) \\
\text{props}(p : \text{cond}_v) &= \{p\}
\end{aligned}$$

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

3.5.3 Describing and validating Wikibase graphs

In this section we present an extension of the ShEx language presented in section 3.5.1 adapted to the wikibase graphs definitions 3.4.4 that we call WShEx.

Definition 3.5.4 — WShEx schema. A *WShEx Schema* is defined as a tuple $\langle \mathcal{L}, \delta \rangle$ where \mathcal{L} set of shape labels, and $\delta : \mathcal{L} \rightarrow \mathcal{S}$ is a total function from labels to w-shape expressions.

The set of w-shape expressions $se \in \mathcal{S}$ is defined using the following abstract syntax. Notice that it is an extension of the abstract syntax for ShEx modifying the rule for triple constraint adding a new element for qualifier specifiers and adding the corresponding rules for qualifier specifiers. The new rules are ²⁴:

²⁴We present the whole abstract syntax in Annex ??

se	$::=$	$cond$	Basic boolean condition on nodes (node constraint)
		$ $ s	Shape
		$ $ se_1 AND se_2	Conjunction
		$ $ se_1 OR se_2	Disjunction
		$ $ NOT se	Negation
		$ $ $@l$	Shape label reference for $l \in \mathcal{L}$
s	$::=$	CLOSED s'	Closed shape
		$ $ s'	Open shape
s'	$::=$	$\{ te \}$	Shape definition
te	$::=$	$te_1; te_2$	Each of te_1 and te_2
		$ $ $te_1 te_2$	Some of te_1 or te_2
		$ $ te^*	Zero or more te
		$ $ $_ \xrightarrow{p} @l qs$	Triple constraint with predicate p value conforming to l and qualifier specifier qs
		$ $ ϵ	Empty triple expression
qs	$::=$	$[ps]$	Open property specifier
		$[ps]$	Closed property specifier
ps	$::=$	ps, ps	<i>EachOf</i> property specifiers
		$ $ $ps ps$	<i>OneOf</i> property specifiers
		$ $ ps^*	zero or more property specifiers
		$ $ ϵ	Empty property specifier
		$ $ $p:@l$	Property p with value conforming to shape l

■ **Example 3.10 — Example of WShEx schema.** A ShEx schema that describes the RDF graph presented in example 3.1 can be defined as:

\mathcal{L}	$=$	$\{ \text{Person, Place, Country, Organization, Date, Award} \}$
$\delta(\text{Person})$	$=$	$\{ _ \xrightarrow{\text{birthDate}} @\text{Date}; _ \xrightarrow{\text{birthPlace}} @\text{Place};$ $_ \xrightarrow{\text{employer}} @\text{Organization} [\text{start} : @\text{Date}, \text{end} : @\text{Date}]^*$ $_ \xrightarrow{\text{awarded}} @\text{Award} [\text{pointTime} : @\text{Date}, \text{togetherWith} : @\text{Person}]^*$ $\}$
$\delta(\text{Place})$	$=$	$\{ _ \xrightarrow{\text{country}} @\text{Country} \}$
$\delta(\text{Country})$	$=$	$\{ \}$
$\delta(\text{Award})$	$=$	$\{ _ \xrightarrow{\text{country}} @\text{Country} \}$
$\delta(\text{Organization})$	$=$	$\{ \}$
$\delta(\text{Date})$	$=$	$\in \text{xsd:date}$

■

The compact syntax for WShEx is similar to ShExC adding the symbols $\{\{ \dots \}$ to declare open qualifier specifiers and $[\{ \dots \}]$ for closed ones.

■ **Example 3.11 — Example of WShEx schema using the compact Syntax.**

```
:Researcher {
  birthPlace    @<Place>          ;
  birthDate     @<Time>           ;
  employer      @<Organization> *
                {{ :start    @:Date ,
                   :end      @:Date
                }} ;
  awarded       @<Award> *
                {{ :pointTime @:Date ,
                   :togetherWith @:Person
                }}
```

```

}
:Place          { country @<Country> }
:Organization   {}
:Award          { country @<Country> }
:Country        {}
:Date           xsd:date

```

■

The semantics of WShEx is based on the semantics of ShEx (see 3.5.1). We present here the changes to the semantics which affect only to the rule that declares conformance to triple constraints. It takes now into account qualifier specifiers²⁵. We declare a new conformance relationship $\mathcal{G}, s, \tau \vdash qs$ between a graph \mathcal{G} a set $s \in P \times V$ of property-value elements, a shape assignment τ and a qualifier specifier qs .

$$\begin{array}{c}
\text{TripleConstraint} \frac{ts = \{\langle x, p, y, s \rangle\} \quad \mathcal{G}, y, \tau \models @l \quad \mathcal{G}, s, \tau \vdash qs}{\mathcal{G}, ts, \tau \models \text{P} @l qs} \\
\\
\text{OpenQs} \frac{s' = \{(p, v) \in s \mid p \in \text{preds}(ps)\} \quad \mathcal{G}, s', \tau \vdash ps}{\mathcal{G}, s, \tau \vdash [ps]} \quad \text{CloseQs} \frac{\mathcal{G}, s, \tau \vdash ps}{\mathcal{G}, s, \tau \vdash [ps]} \\
\\
\text{EachOfQs} \frac{\mathcal{G}, s, \tau \vdash ps_1 \quad \mathcal{G}, s, \tau \vdash ps_2}{\mathcal{G}, s, \tau \vdash ps_1, ps_2} \\
\\
\text{OneOfQs}_1 \frac{\mathcal{G}, s, \tau \vdash ps_1}{\mathcal{G}, s, \tau \vdash ps_1 \mid ps_2} \quad \text{OneOfQs}_2 \frac{\mathcal{G}, s, \tau \vdash ps_2}{\mathcal{G}, s, \tau \vdash ps_1 \mid ps_2} \\
\\
\text{StarQs}_1 \frac{}{\mathcal{G}, \emptyset, \tau \vdash ps^*} \quad \text{StarQs}_2 \frac{(s_1, s_2) \in \text{part}(s) \quad \mathcal{G}, s_1, \tau \vdash ps \quad \mathcal{G}, s_2, \tau \vdash ps^*}{\mathcal{G}, s, \tau \vdash ps^*} \\
\\
\text{EmptyQs} \frac{}{\mathcal{G}, \emptyset, \tau \vdash \epsilon} \quad \text{PropertyQs} \frac{s = \{(p, v)\} \quad \mathcal{G}, v, \tau \models @l}{\mathcal{G}, s, \tau \vdash p : @l}
\end{array}$$

3.6 Knowledge Graphs Subsets

Esta sección es un borrador de ideas todavía...

In this section we will review different approaches to create subsets of knowledge graphs.

We will focus mainly on Wikidata subsets although the approaches could also be applied to RDF-based graphs and property graphs.

3.6.1 Wikibase Subsets: Formal definition

The following definition of Wikibase subset is based on the definition of wikibase graphs given at section 3.4.3.

Definition 3.6.1 — Wikibase subset. Given a wikibase graph $\mathcal{G} = \langle \mathcal{Q}, \mathcal{P}, \mathcal{D}, \mathcal{S} \rangle$, a wikibase subgraph is defined as $\mathcal{G}' = \langle \mathcal{Q}', \mathcal{P}', \mathcal{D}', \mathcal{S}' \rangle$ such that: $\mathcal{Q}' \subseteq \mathcal{Q}$, $\mathcal{P}' \subseteq \mathcal{P}$, $\mathcal{D}' \subseteq \mathcal{D}$ and $\mathcal{S}' \subseteq \mathcal{S}$

■ **Example 3.12 — Example of wikibase subgraph.** Given the wikibase graph from example 3.4

²⁵The full inference rules of WShEx semantics are presented in Annex ??

$\mathcal{G}' = \langle \mathcal{Q}', \mathcal{P}', \mathcal{D}', \mathcal{S}' \rangle$ where

$$\begin{aligned}\mathcal{Q}' &= \{\text{timBl}, \text{London}, \text{CERN}\} \\ \mathcal{P}' &= \{\text{birthPlace}, \text{employer}, \text{start}\} \\ \mathcal{D}' &= \{1980, 1984\} \\ \mathcal{S}' &= \{(\text{timBl}, \text{birthPlace}, \text{London}, \{\}), \\ &\quad (\text{timBl}, \text{employer}, \text{CERN}, \{\text{start} : 1980\}), \\ &\quad (\text{timBl}, \text{employer}, \text{CERN}, \{\text{start} : 1984\})\}\end{aligned}$$

is a wikibase subgraph of \mathcal{G} . ■

3.6.2 Generating subgraphs from subsets of items or properties

Wikibase subgraphs can be generated from a set of items or properties, where we collect the subgraph associated with those entities.

Definition 3.6.2 — Item-generated subgraph. Given a wikibase graph $\mathcal{G} = \langle \mathcal{Q}, \mathcal{P}, \mathcal{D}, \mathcal{S} \rangle$ and a subset of items $\mathcal{Q}_s \subset \mathcal{Q}$ generates an *item-generated subgraph* $\langle \mathcal{Q}', \mathcal{P}', \mathcal{D}', \mathcal{S}' \rangle$ such that:

$$\begin{aligned}\mathcal{Q}' &= \{q \in \mathcal{Q} \mid (q, _, _, _) \vee (_, _, q, _) \in \mathcal{S}'\} \\ &\quad \cup \{q \in \mathcal{Q} \mid (_, _, _, q_s) \in \mathcal{S}' \wedge (_, q) \in q_s\} \\ \mathcal{P}' &= \{p \in \mathcal{P} \mid (_, p, _, _) \in \mathcal{S}'\} \\ &\quad \cup \{p \in \mathcal{P} \mid (_, _, _, q_s) \in \mathcal{S}' \wedge (p, _) \in q_s\} \\ \mathcal{D}' &= \{d \in \mathcal{D} \mid (_, _, d, _) \in \mathcal{S}'\} \\ &\quad \cup \{d \in \mathcal{D} \mid (_, _, _, q_s) \in \mathcal{S}' \wedge (_, d) \in q_s\} \\ \mathcal{S}' &= \{(q, _, _, _) \in \mathcal{S} \mid q \in \mathcal{Q}_s\} \\ &\quad \cup \{(_, _, q, _) \in \mathcal{S} \mid q \in \mathcal{Q}_s\} \\ &\quad \cup \{(_, _, _, q_s) \in \mathcal{S} \wedge \exists q \in \mathcal{Q}_s \mid (_, q) \in q_s\}\end{aligned}$$

Notice that the item-generated subgraph usually contains more items than the items provided by \mathcal{Q}_s .

■ **Example 3.13 — Example of item-generated subgraph.** Given the wikibase graph from example 3.4 and $\mathcal{Q}_s = \{\text{timBl}\}$ the item generated subgraph is:

$$\begin{aligned}\mathcal{Q}' &= \{\text{timBl}, \text{CERN}, \text{vintCerf}, \text{PA}\} \\ \mathcal{P}' &= \{\text{birthDate}, \text{birthPlace}, \text{employer}, \text{awarded}, \\ &\quad \text{start}, \text{end}, \text{togetherWith}\} \\ \mathcal{D}' &= \{1984, 1994, 1980, 1955\} \\ \mathcal{S}' &= \{(\text{timBl}, \text{birthDate}, 1955, \{\}), \\ &\quad (\text{timBl}, \text{birthPlace}, \text{London}, \{\}), \\ &\quad (\text{timBl}, \text{employer}, \text{CERN}, \{\text{start} : 1980, \text{end} : 1980\}), \\ &\quad (\text{timBl}, \text{employer}, \text{CERN}, \{\text{start} : 1984, \text{end} : 1994\}), \\ &\quad (\text{timBl}, \text{awarded}, \text{PA}, \{\text{togetherWith} : \text{vintCerf}\}), \\ &\quad (\text{vintCerf}, \text{awarded}, \text{PA}, \{\text{togetherWith} : \text{timBl}\})\}\end{aligned}$$

■

Definition 3.6.3 — Property-generated subgraph. Given a wikibase graph $\mathcal{G} = \langle \mathcal{Q}, \mathcal{P}, \mathcal{D}, \mathcal{S} \rangle$, with the set of entities $\mathcal{E} = \mathcal{Q} \cup \mathcal{P}$ a subset of properties $\mathcal{P}_s \subset \mathcal{P}$ generates a *property generated subgraph* $\langle \mathcal{Q}', \mathcal{P}', \mathcal{D}', \mathcal{S}' \rangle$ such that:

$$\begin{aligned} \mathcal{Q}' &= \{q \in \mathcal{Q} \mid \exists p \in \mathcal{P}_s \mid (q, p, _, _) \in \mathcal{S}\} \\ &\quad \cup \{q \in \mathcal{Q} \mid \exists p \in \mathcal{P}_s \mid (_, p, q, _) \in \mathcal{S}\} \\ &\quad \cup \{q \in \mathcal{Q} \mid (_, _, _, q_s) \in \mathcal{S} \wedge \exists p \in \mathcal{P}_s \mid (p, _) \in q_s\} \\ \mathcal{P}' &= \{p \in \mathcal{P}_s \mid (_, p, _, _) \in \mathcal{S}\} \\ &\quad \cup \{p \in \mathcal{P}_s \mid \exists q_s \mid (_, _, _, q_s) \in \mathcal{S} \wedge (p, _) \in q_s\} \\ \mathcal{D}' &= \{d \in \mathcal{D} \mid \exists p \in \mathcal{P}_s \mid (_, p, d, _) \in \mathcal{S}\} \\ &\quad \cup \{d \in \mathcal{D} \mid (_, _, _, q_s) \in \mathcal{S} \wedge \exists p \in \mathcal{P}_s \mid (p, d) \in q_s\} \\ \mathcal{S}' &= \{(_, p, _, _) \in \mathcal{S} \mid p \in \mathcal{P}_s\} \\ &\quad \cup \{(_, _, _, q_s) \in \mathcal{S} \mid \exists p \in \mathcal{P}_s \mid (p, _) \in q_s\} \end{aligned}$$

The property generated subgraph usually contains more properties than the properties provided by \mathcal{P}_s .

■ **Example 3.14 — Example of property-generated subgraph.** Given the wikibase graph from example 3.4 and $\mathcal{P}_s = \{\text{birthDate}, \text{togetherWith}\}$ the property generated subgraph is:

$$\begin{aligned} \mathcal{Q}' &= \{\text{timBl}, \text{vintCerf}, \text{PA}\} \\ \mathcal{P}' &= \{\text{birthDate}, \text{awarded}, \text{togetherWith}\} \\ \mathcal{D}' &= \{1955\} \\ \mathcal{S}' &= \{(\text{timBl}, \text{birthDate}, 1955, \{\}), \\ &\quad (\text{timBl}, \text{awarded}, \text{PA}, \{\text{togetherWith} : \text{vintCerf}\}), \\ &\quad (\text{vintCerf}, \text{awarded}, \text{PA}, \{\text{togetherWith} : \text{timBl}\})\} \end{aligned}$$

■

Notice that it is possible to define a *Datatype-generated subgraph* in a similar way than the previous definitions.

Definition 3.6.4 — Entity-generated subgraph. Given a subset of entities $\mathcal{E}_s \subset \mathcal{Q} \cup \mathcal{P}$, the entity-generated subgraph is defined as the union of the item-generated subgraph with all the items in \mathcal{E}_s and the property-generated subgraph with all the properties in \mathcal{E}_s .

3.6.3 Graph matching

Definition 3.6.5 — Matching expression. Given a wikibase graph $\mathcal{G} = \langle \mathcal{Q}, \mathcal{P}, \mathcal{D}, \mathcal{S} \rangle$ where $\mathcal{E} = \mathcal{Q} \cup \mathcal{P}$ and $\mathcal{V} = \mathcal{E} \cup \mathcal{D}$, a matching expression M_s is a set of matchers where each matcher m follows the grammar:

m ::=	subject(e)	Subject $e \in \mathcal{E}$
	property(p)	Property $p \in \mathcal{P}$
	value(v)	Value $v \in \mathcal{V}$
	qualifier(p,v)	Qualifier with property $p \in \mathcal{P}$ and value $v \in \mathcal{V}$
	qualifiedProp(p)	Qualifier with property $p \in \mathcal{P}$
	qualifiedValue(v)	Qualifier with value $v \in \mathcal{V}$

■ **Example 3.15 — Example of a matcher expression.** An example of a matcher expression is $M_s = \{\text{property}(\text{country}), \text{qualifiedProp}(\text{togetherWith})\}$ ■

Definition 3.6.6 — Matching-generated subgraph. Given a matching expression M_s over a wikibase graph $\mathcal{G} = \langle \mathcal{Q}, \mathcal{P}, \mathcal{D}, \mathcal{S} \rangle$ we can define the matching-generated subgraph as a wikibase graph $\mathcal{G}' = \langle \mathcal{Q}', \mathcal{P}', \mathcal{D}', \mathcal{S}' \rangle$ such that:

$$\begin{aligned}
 \mathcal{Q}' &= \{q \in \mathcal{Q} \mid (q, _, _, _) \in \mathcal{S}' \cup \{q \in \mathcal{Q} \mid (_, _, q, _) \in \mathcal{S}'\} \\
 &\quad \cup \{q \in \mathcal{Q} \mid (_, _, _, q_s) \in \mathcal{S}' \wedge (_, q) \in q_s\} \\
 \mathcal{P}' &= \{p \in \mathcal{P} \mid (_, p, _, _) \in \mathcal{S}' \cup \{p \in \mathcal{P} \mid (_, _, _, q_s) \in \mathcal{S}' \wedge (p, _) \in q_s\} \\
 \mathcal{D}' &= \{d \in \mathcal{D} \mid (_, _, d, _) \in \mathcal{S}'\} \cup \{d \in \mathcal{D} \mid (_, _, _, q_s) \in \mathcal{S}' \wedge (_, d) \in q_s\} \\
 \mathcal{S}' &= \{(q, _, _, _) \in \mathcal{S} \mid \text{subject}(q) \in M_s\} \\
 &\quad \cup \{(_, p, _, _) \in \mathcal{S} \mid \text{property}(p) \in M_s\} \\
 &\quad \cup \{(_, _, v, _) \in \mathcal{S} \mid \text{value}(v) \in M_s\} \\
 &\quad \cup \{(_, _, _, q_s) \in \mathcal{S} \mid \text{qualifier}(p, v) \in M_s \wedge \exists (p, v) \in q_s\} \quad \cup \{(_, _, _, q_s) \in \mathcal{S} \mid \text{qualifiedProp}(p) \in M_s\}
 \end{aligned}$$

■ **Example 3.16 — Example of matching-generated subgraph.** Given the wikibase graph \mathcal{G} of example 3.4 and the matching-expression M_s in example ??, the matching-generated subgraph of \mathcal{G} from M_s is the wikibase graph $\mathcal{G}' = \langle \mathcal{Q}', \mathcal{P}', \mathcal{D}', \mathcal{S}' \rangle$ such that:

$$\begin{aligned}
 \mathcal{Q}' &= \{\text{PA}, \text{Spain}, \text{London}, \text{UK}, \text{timBl}, \text{vintCerf}\} \\
 \mathcal{P}' &= \{\text{country}, \text{awarded}, \text{togetherWith}\} \\
 \mathcal{D}' &= \{\} \\
 \mathcal{S}' &= \{(\text{timBl}, \text{awarded}, \text{PA}, \{\text{togetherWith} : \text{vintCerf}\}), \\
 &\quad (\text{vintCerf}, \text{awarded}, \text{PA}, \{\text{togetherWith} : \text{timBl}\}) \\
 &\quad (\text{PA}, \text{country}, \text{Spain}, \{\}) \\
 &\quad (\text{London}, \text{country}, \text{UK}, \{\})\}
 \end{aligned}$$

This approach is followed by WDumper²⁶.

It consists of matching each triple with a target specification of the expected contents.

the approach
the running exam-

3.6.4

ShEx Slurping

Keep track of the matched triples while validating.

Create a new semantics of Shape Expressions that generates slurps while validating...

²⁶<https://github.com/bennofs/wdumper>

This approach has been implemented by PyShEx²⁷ and ShEx.js²⁸ implementations.

This approach may be difficult to scale as it is validating at the same time that it is doing the slurping process. Validating complexity is high because it may require to check the different partitions of a node neighbourhood.

3.6.5 Flatten ShEx + Slurping

It is possible to identify ShEx subsets that enable faster validation. One such subset that we name flatten ShEx defines triple expressions as follows:

3.6.6 ShEx based traversal using Pregel

Pregel [41] has been proposed as an scalable computational model created by Google to handle large graphs. It is based on Bulk Synchronous Parallel (BSP) model which simplifies parallel programming having different computation and communication phases. Pregel is an iterative algorithm where each phase is called a superstep. Following the lemma *think like a vertex*, it is a vertex-centric abstraction where at each superstep, a vertex executes a user defined function (called vertex program) which can update its status and later sends messages to neighbors along graph edges. Supersteps end with a synchronization barrier that guarantees that messages sent at one superstep are received at the beginning of the next superstep. Vertices may change status between active and inactive and the algorithm terminates when all vertices are inactive and no more messages are sent.

GraphX was proposed in 2014 as a graph processing framework embedded in Apache Spark. Its API includes a variant of Pregel which is used to implement several graph algorithms like PageRank, connected components, triangle counting, etc.

GraphX defines an API for graphs based on RDDs (resilient distributed datasets). An $\text{RDD}[\mathcal{V}]$ is an abstraction of a collection of values of type \mathcal{V} which are immutable and can be partitioned to run data-parallel operations like *map* and *reduce*.

A graph $\text{Graph}[\mathcal{V}, \mathcal{E}]$ represents an abstraction of vertices with values of type \mathcal{V} and edges of type \mathcal{E} where internally the vertices are represented as $\text{RDD}[(\text{Id}, \mathcal{V})]$, i.e. a collection of a tuple with an Id (a Long value) and a \mathcal{V} , and edges are represented as $\text{RDD}[(\text{Id}, \text{Id}, \mathcal{E})]$, i.e. a triple where the first and second components are the Id of the source and destiny respectively, and the third component is the edge property $p \in \mathcal{E}$. A graph $\text{Graph}[\mathcal{V}, \mathcal{E}]$ also provides what is called a *triplets* view which represents edges as collections of triplets of the form $\text{RDD}[(\mathcal{V}, \mathcal{E}, \mathcal{V})]$. A triplet t will be denoted by the type `Triplet` and provides access to the source vertex (using `t.srcAttr`), the destiny (`t.dstAttr`) and the edge property (`t.attr`).

GraphX provides several built-in operators for graphs²⁹. We will use the following in the rest of the paper:

- `mapVertices(g: Graph[\mathcal{V}, \mathcal{E}], f: (Id, \mathcal{V}) \rightarrow \mathcal{V}): Graph[\mathcal{V}, \mathcal{E}]` maps every pair (id, v) in the vertices of g to ($\text{id}, f(v)$).
- `mapReduceTriples(g: Graph[\mathcal{V}, \mathcal{E}], m: ($\mathcal{V}, \mathcal{E}, \mathcal{V}$) \rightarrow [(Id, \mathcal{M})], r: (\mathcal{M}, \mathcal{M}) \rightarrow \mathcal{M}): RDD[(Id, \mathcal{M})]`, encodes the two-stage parallel computation process commonly known as mapReduce using the triplets view. It takes as parameters, a graph g , a map function m and a reduce function r .

In the first stage it applies the m to each triplet in the graph to generate a list of messages that will be sent to the vertices identified a given id .

In the second stage, it groups all the messages sent to a given vertex applying the reduce function r to each pair of messages.

²⁷<https://github.com/hsolbrig/PyShEx>

²⁸<https://github.com/shexjs/shex.js>

²⁹<https://spark.apache.org/docs/latest/graphx-programming-guide.html>

- $\text{joinVertices}(g:\text{Graph}[\mathcal{V},\mathcal{E}], \text{msgs}:\text{RDD}[(\text{Id}, \mathcal{M})], f:(\text{Id}, \mathcal{V}, \mathcal{M}) \rightarrow \mathcal{V}): \text{Graph}[\mathcal{V},\mathcal{E}]$, joins the collection of messages sent to a the vertices which have a value (id, m) with the vertex v identified by id and replaces that vertex by $f(\text{id}, v, m)$.

The GraphX Pregel algorithm is defined iteratively where each iteration is usually called a superstep as follows:

Algorithm 1: Pregel algorithm pseudocode as implemented in GraphX

Input parameters:

$g: \text{Graph}[\mathcal{V}, \mathcal{E}]$
 $\text{initialMsg}: \mathcal{M}$
 $\text{vProg}: (\text{Id}, \mathcal{V}, \mathcal{M}) \rightarrow \mathcal{V}$
 $\text{sendMsg}: \text{Triplet} \rightarrow [(\text{Id}, \mathcal{M})]$
 $\text{mergeMsg}: (\mathcal{M}, \mathcal{M}) \rightarrow \mathcal{M}$

Output: $g: \text{Graph}[\mathcal{V}, \mathcal{E}]$

```

1  $g = \text{mapVertices}(g, \lambda(\text{id}, v) \rightarrow \text{vProg}(\text{id}, v, \text{initialMsg}))$ 
2  $\text{msgs} = \text{mapReduceTriples}(g, \text{sendMsg}, \text{mergeMsg})$ 
3 while  $\text{size}(\text{msgs}) > 0$  do
4    $g = \text{joinVertices}(g, \text{msgs}, \text{vProg})$ 
5    $\text{msgs} = \text{mapReduceTriples}(g, \text{sendMsg}, \text{mergeMsg})$ 
6 return  $g$ 

```

It takes as input a $\text{Graph}[\mathcal{V}, \mathcal{E}]$ and the following parameters:

- initialMsg : initial message sent to all the vertices
- vprog is the vertex program. It is run by each vertex at the beginning of the algorithm using the initialMsg and in each superstep using the collected messages sent by the neighbors in the previous superstep.
- sendMsg takes as parameter an triplet and returns an iterator with a pair (id, msg) where id represents the id of the vertex which will receive the message and msg represents the message that will be sent.
- mergeMsg is a function that defines how to merge 2 messages into one. This function must be associative and commutative, and will be invoked to collect all the messages that are sent to a vertex in each superstep.

We have implemented a ShEx validation algorithm based on the Pregel algorithm. The algorithm assumes that there is a ShEx schema $\langle \mathcal{L}, \delta \rangle$ where each label $l \in \mathcal{L}$ identifies a shape expression.

The algorithm annotates each node $n \in \mathcal{V}$ with a status map that represents the validation status with regards to some labels. The new nodes in the graph will be tuples (n, m) where $n \in \mathcal{V}$, and $m: \mathcal{L} \mapsto \text{Status}$ associates a status for each shape label.

A Status is defined as:

Status ::= Undefined	Default status
Ok	Node conforms
Failed	Node doesn't conform
Pending	Requested to conform
WaitingFor(ds, oks, fs)	Waiting for some neighbours
	ds = list dependants neighbours
	oks = list of conformant neighbours
	fs = list of non conformant neighbours
	where ds, oks, failed $\in \mathcal{V} \times \mathcal{P} \times \mathcal{L}$

The status can be Undefined if there is no information yet (this is the default value) Ok if the node conforms to the shape identified by l , Failed if it doesn't conform to the shape, Pending if

the node has been requested to be validated with that label or `WaitingFor(ds, oks, failed)` if the validation of node n depends on the validation of a set of neighbour nodes ds . Each neighbour node is represented by a triple (v, p, l) where v is the neighbour node, p is the property which links n with v , and l is the shape label that the node must conform. During the validation, we may receive information that some of those neighbour nodes have been validated or failed. That information is collected in the set `oks` which is the set of conforming neighbour nodes and `failed` is the set of failed neighbour nodes.

A message can be represented as a map which assigns to each label the following requests:

<code>Msg ::= Validate</code>	Request to validate
<code> Checked(oks, fs)</code>	Some neighbours have been checked oks = neighbours that have been checked as conformant fs = neighbours that have been checked as non-conformant where $oks, fs \in \mathcal{V} \times \mathcal{P} \times \mathcal{L}$
<code> WaitFor(ds)</code>	Request to wait for some neighbours where $ds \in \mathcal{V} \times \mathcal{P} \times \mathcal{L}$

The Pregel-ShEx-validation traversal is defined with the following pseudocode.

Algorithm 2: Pregel-based ShEx validation pseudocode

Input parameters:

```

g: Graph[ $\mathcal{V}$ ,  $\mathcal{E}$ ]
initialLabel:  $\mathcal{L}$ 
checkLocal: ( $\mathcal{L}$ ,  $\mathcal{V}$ )  $\rightarrow$  Ok|Failed|Pending(Set[ $\mathcal{L}$ ])
checkNeighs: ( $\mathcal{L}$ , Bag[( $\mathcal{E}$ ,  $\mathcal{L}$ )], Set[( $\mathcal{E}$ ,  $\mathcal{L}$ )])  $\rightarrow$  Ok|Failed
tripleConstraints:  $\mathcal{L} \rightarrow$  Set[( $\mathcal{E}$ ,  $\mathcal{L}$ )]

```

Output: $g: \text{Graph}[(\mathcal{V}, \mathcal{L} \mapsto \text{Status}), \mathcal{E}]$

```

gs = mapVertices(g,  $\lambda(id, v) \rightarrow (id, (v, \lambda v \rightarrow \text{Undefined}))$ )
gs = pregel(Validate, gs, vProg, sendMsg, mergeMsg)
gs = mapVertices(gs, checkUnsolved)
return gs

```

def checkUnsolved(v, m) = (v, m') where

$$m'(l) = \begin{cases} \text{checkNeighs}(l, \emptyset, \emptyset) & \text{if } m(l) = \text{Pending} \\ \text{checkNeighs}(l, oks, fs \cup ds) & \text{if } m(l) = \text{WaitingFor}(ds, oks, fs) \\ m(l) & \text{otherwise} \end{cases}$$

def vProg: ($\text{Id}, \mathcal{V}, \mathcal{M}$) $\rightarrow \mathcal{V} = \dots$ see 9

The algorithm takes as input the parameters:

- `initialLabel` is the initial shape label that is requested to validate every node in the graph. In Shape Expressions, this label is usually annotated with the `start` keyword.
- `checkLocal` checks if the shape expression associated with a label can validate a node locally. It returns `Ok` if the node validates without further dependencies, `Failed`, if it doesn't validate, and `Pending(ls)` if the validation of the node depends on a list of shape labels `ls`.
- `checkNeighs` checks if the bag of neighbors of a node matches the regular bag expression associated with the label in the schema.
- `tripleConstraints` returns the list of triple constraints associated with the shape expression indicated by the label.

The algorithm starts by mapping every node to the status which associates any label $l \in \mathcal{L}$ to undefined (`Undefined`). After that, it runs the iterative Pregel algorithm using the `vProg`, `sendMsg` and `mergeMsg` functions defined as above. Once the Pregel algorithm finishes, it replaces the status

$\frac{(n, m), l \rightsquigarrow \text{Validate} \quad m(l) = s \in \{\text{Undefined}, \text{Pending}\} \quad \text{checkLocal}(l, n) = r \in \{\text{Ok}, \text{Failed}\}}{m'(l) = r}$
$\frac{(n, m), l \rightsquigarrow \text{Validate} \quad m(l) = r \in \{\text{Undefined}, \text{Pending}\} \quad \text{checkLocal}(l, n) = \text{Pending}(ls)}{m'(l) = \text{Undefined} \quad m'(l') = \text{Pending} \forall l' \in ls}$
$\frac{(n, m), l \rightsquigarrow \text{Validate} \quad m(l) = r \in \{\text{Ok}, \text{Failed}\}}{m'(l) = r}$
$\frac{(n, m), l \rightsquigarrow \text{Validate} \quad m(l) = \text{WaitingFor}(ds, oks, fs)}{m'(l) = \text{Ok}}$
$\frac{(n, m), l \rightsquigarrow \text{Checked}(oks, fs) \quad m(l) = \text{WaitingFor}(ds, oks', fs') \quad ds \setminus (oks \cup fs) \neq \emptyset}{m'(l) = \text{WaitingFor}(ds, oks \cup oks', fs \cup fs')}$
$\frac{(n, m), l \rightsquigarrow \text{Checked}(oks, fs) \quad m(l) = \text{WaitingFor}(ds, oks', fs') \quad ds \setminus (oks \cup fs) = \emptyset}{m'(l) = \text{checkNeighs}(l, oks \cup oks', fs \cup fs')}$

Table 3.1: Definition of v_{Prog} for Pregel-based ShEx validation

of any node that is pending or waiting for some neighbours by a last check based on the current information of the neighbours, assuming that if the node didn't receive information that a pending neighbour has validated, it means that there was no evidence of its validation, and it failed.

v_{Prog} changes the status map of a node with regards to a label when it receives a message for that label. It can be defined as:

$v_{\text{Prog}}(\text{id}, (n, m), \text{msg}) = (n, m')$ where $m'(l) = m(l)$ except for the cases indicated by the following rules:

Figure 3.6 represents a state diagram which shows the different status that a node can have with regards to a shape label. Initially, all nodes have status `Undefined` until they get a message request to validate against some label. If it is possible to validate locally those nodes, then they will go directly to the end state which can be `Ok` or `Failed`. Otherwise, if their validation depends on the neighbours, they will enter the status `Pending` whose nodes are active in the Pregel algorithm and will be activated in the messages generation phase. If they receive a request to wait for some other nodes to be validated, they will go to the state `WaitingFor(ds, oks, fs)` which means that they are waiting for the status of the neighbour nodes `ds`.

In subsequent phases, they can receive notifications that some of those neighbour nodes have either been validated or not updating the corresponding values of `oks` and `fs`. Once all the pending neighbours have either been validated or failed, it will invoke `checkNeighs(l, oks, fs)` to check if the regular expression matches taking into account which neighbours conform or don't conform and passing to the state `Ok` or `Failed` which is inactive.

Once executed the Pregel algorithm, it is possible that some nodes are in state `Pending` and don't receive any message, which means that their validation depends on the existence of some arcs

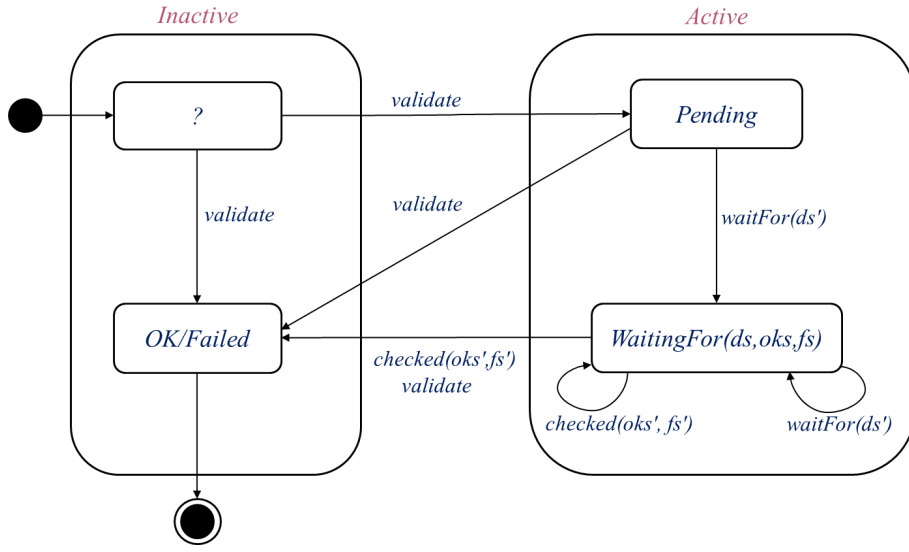


Figure 3.6: State diagram representing the different states in vProg

$\frac{\langle (s, m_s), p, (o, m_o) \rangle \in \mathcal{G} \quad m_s(l) = \text{Pending} \quad \text{tcs}(l, \mathcal{S}) = \perp \xrightarrow{p} @l'}{(s, m_s), l \rightsquigarrow \text{WaitFor}((o, p, l')) \quad (o, m_o), l \rightsquigarrow \text{Validate}}$			
$\frac{\langle (s, m_s), p, (o, m_o) \rangle \in \mathcal{G} \quad m_s(l) = \text{WaitingFor}(ds, oks, fs) \quad (o, p, l') \in ds \quad m_o(l') = \text{Ok}}{(s, m_s), l \rightsquigarrow \text{Checked}((o, p, l'), \emptyset)}$			
$\frac{\langle (s, m_s), p, (o, m_o) \rangle \in \mathcal{G} \quad m_s(l) = \text{WaitingFor}(ds, oks, fs) \quad (o, p, l') \in ds \quad m_o(l') = \text{Failed}}{(s, m_s), l \rightsquigarrow \text{Checked}(\emptyset, (o, p, l'))}$			

Table 3.2: Definition of `sendMsg` for Pregel-based ShEx validation

pointing to some neighbours and they didn't receive messages from those arcs, i.e. there are no arcs in the graph. In that case, a last step in the algorithm checks if those nodes can validate with an empty neighbourhood.

The messages that are sent in the message generation phase are defined using the following presented in table 9.

In order to define `sendMsg(Triplet):[(Id,Msg)]` we will use the notation $(x, m_x), l \rightsquigarrow \text{Msg}$ to represent that message `Msg` is sent to the node x with satsus map m_x for label l . Table 9 represents the rules that declare which messages are sent for each triplet view which is represented as $\langle (s, m_s), p, (o, m_o) \rangle$ where (s, m_s) is the subject, p the predicate and (o, m_o) the object:

Finally `mergeMsg` merges the messages that arrive to the same node and can be defined as:

$$\text{mergeMsg}((n, m), l \rightsquigarrow \text{msg}_1, (n, m), l \rightsquigarrow \text{msg}_2) = (n, m), l \rightsquigarrow \text{msg}_1 \oplus \text{msg}_2$$

where

$$\begin{aligned}
\text{Validate} \oplus y &= y \\
\text{Validate} \oplus \text{Checked}(oks, fs) &= \text{Checked}(oks, fs) \\
\text{Validate} \oplus \text{WaitFor}(ds) &= \text{WaitFor}(ds) \\
\text{Checked}(oks, fs) \oplus \text{Validate} &= \text{Checked}(oks, fs) \\
\text{Checked}(oks, fs) \oplus \text{Checked}(oks', fs') &= \text{Checked}(oks \cup oks', fs \cup fs') \\
\text{Checked}(oks, fs) \oplus \text{WaitFor}(ds) &= \text{Checked}(oks \cup ds, fs \cup fs) \\
\text{WaitFor}(ds) \oplus \text{Validate} &= \text{WaitFor}(ds) \\
\text{WaitFor}(ds) \oplus \text{Checked}(oks, fs) &= \text{Checked}(oks \cup ds, fs) \\
\text{WaitFor}(ds) \oplus \text{WaitFor}(ds') &= \text{WaitFor}(ds \cup ds')
\end{aligned}$$

The algorithm presented in figure 2 required as parameters a function $\text{checkLocal}: (\mathcal{L}, \mathcal{V}) \rightarrow \text{Ok} | \text{Failed} | \text{Pending}(\text{Set}[\mathcal{L}])$ that returns Ok if it is possible to check that the node conforms to a shape label locally, Failed if it is possible to check that a node doesn't conform to a shape label locally, and Pending(ls) if the conformance of a node depends on the arcs in ls.

Figure 3 presents a possible implementation of checkLocal for WShEx.

Algorithm 3: Definition of checkLocal for a WShEx schema $\langle \mathcal{L}, \delta \rangle$ and wikibase graph $\mathcal{G} = \langle \rho \rangle$

```

def  $\text{checkLocal}(l, (n, m)) = \text{checkLocal}(\delta(l), (n, m))$ 
def  $\text{checkLocal}(se, (n, m)) = \text{match } se$ 
  case  $se_1 \text{ AND } se_2 \Rightarrow \text{checkLocal}(se_1, (n, m)) \wedge \text{checkLocal}(se_2, (n, m))$ 
  case  $se_1 \text{ OR } se_2 \Rightarrow \text{checkLocal}(se_1, (n, m)) \vee \text{checkLocal}(se_2, (n, m))$ 
  case  $\text{NOT } se \Rightarrow \neg \text{checkLocal}(se, (n, m))$ 
  case  $@l \Rightarrow \text{checkLocal}(\delta(l), (n, m))$ 
  case  $\text{CLOSED? } \{ te \} \Rightarrow \text{let}$ 
     $(oks, fs) = \text{checkLocalOpen}(te, \text{neighs}(m, n))$ 
     $s_2 = \text{if } \text{CLOSED} \text{ then}$ 
       $\perp \quad fs = \emptyset$ 
    else
      in  $\text{todo} \dots$ 
def  $\text{checkLocalOpen}(te, (n, m)) = \text{match } te$ 
  case  $te_1; te_2 \Rightarrow \text{checkLocalOpen}(te_1, (n, m)) \wedge \text{checkLocalOpen}(te_2, (n, m))$ 
  case  $te_1 | te_2 \Rightarrow \text{checkLocalOpen}(te_1, (n, m)) \vee \text{checkLocalOpen}(te_2, (n, m))$ 
  case  $\perp \xrightarrow{p} @l\{\min, \max\} \Rightarrow \text{Pending} \mid \text{case } \perp \xrightarrow{p} \text{cond}\{\min, \max\} \Rightarrow \text{cond}(m)$ 

```

$\text{checkNeighs}: (\mathcal{L}, \text{Bag}[(\mathcal{E}, \mathcal{L})], \text{Set}[(\mathcal{E}, \mathcal{L})]) \rightarrow \text{Ok} | \text{Failed}$ can be implemented as in figure ??.

Algorithm 4: Definition of checkNeighs for a WShEx schema $\langle \mathcal{L}, \delta \rangle$ and wikibase graph $\mathcal{G} = \langle \mathcal{Q}, \mathcal{P}, \mathcal{D}, \rho \rangle$

```

def  $\text{checkNeighs}(l, bag, fs) = \text{checkNeighs}(\delta(l), bag, fs)$ 
def  $\text{checkNeighs}(se, bag, fs) = \text{match } se$ 
  case  $se_1 \text{ AND } se_2 \Rightarrow \text{checkNeighs}(se_1, bag, fs) \wedge \text{checkNeighs}(se_2, bag, fs)$ 
  case  $se_1 \text{ OR } se_2 \Rightarrow \text{checkNeighs}(se_1, bag, fs) \vee \text{checkNeighs}(se_2, bag, fs)$ 
  case  $\text{NOT } se \Rightarrow \neg \text{checkNeighs}(se, bag, fs)$ 
  case  $@l \Rightarrow \text{checkNeighs}(\delta(l), bag, fs)$ 
  case  $\text{CLOSED? } \{ te \} \Rightarrow \text{matchRbe}(bag, \text{rbe}(te))$ 

```

Finally, the parameter $\text{tripleConstraints}: \mathcal{L} \rightarrow \text{Set}[(\mathcal{E}, \mathcal{L})]$ is defined in figure ??

3.6.7 Representing Wikidata in Spark GraphX

Spark GraphX supports a kind of property graphs where vertices and edges can have an associated value. The type `Graph[VD,ED]` is used to represent a graph whose vertices are pairs of values of type `(VertexId,VD)` where `VertexId=Long` represents a unique vertex identifier and `VD` represents the value associated with the vertex.

When representing Wikidata graphs in Spark GraphX it is necessary to take into account which entities will be represented as vertices. We opted to include as nodes in the graph only those nodes that can be subjects of statements, i.e. wikidata entities (items and properties), leaving out primitive values like literals, dates, etc. We separated the statements associated with an entity in two kind of statements: local statements, which are embedded inside the value of a node and whose values can be accessed without traversing the graph, and entity statements, whose values are other entities which have their corresponding vertex in the graph.

In this way, the WShEx also needs to distinguish triple expressions between local ones and entity ones.

3.7 Use cases and Applications

In this section we describe some use cases and applications where generating wikidata subsets is necessary.

3.7.1 Scholia

Scholia is a project that is based on visualizing scientific information from Wikidata [52]³⁰. It offers visualizations about researcher's contributions which are currently generated from direct SPARQL queries to the Wikidata Query Service.

Given the size of Wikidata, visualizations that need to be obtained from large number of results can not be shown for several reasons:

- The queries require a lot of intermediate results which can not be manipulated
- The complexity of the queries require more time than the time slot provided by the wikidata query service.
- ...

As an example, the aspect that visualizes authors by country only works for small countries.

talk a bit more about this so we can later include experiment results...

3.7.2 GeneWiki project

The GeneWiki project has been used as an running example with domain-specific data to generate wikidata subsets in [38].

Talk more about this...compounds example?

3.8 Results

3.9 Related work

Knowledge graphs

An introduction to Knowledge graphs is provided by [29], which cites other books [19, 32, 55] and surveys like [2, 21, 56, 71, 72, 73]. In this paper, we follow the graph models provided in that survey: directed labeled graphs and property graphs and add a new one: wikibase graphs.

³⁰<https://scholia.toolforge.org/>

KGRAM (Knowledge Graph Abstract Machine) [12] defines a framework for querying knowledge graphs in different models.

Knowledge graph descriptions

Since the appearance of ShEx in 2014, there has been a lot of interest about RDF validation and description. In 2017, the data shapes working group proposed SHACL (Shapes Constraint Language) as a W3C recommendation [34]. Although SHACL can be used to describe RDF, its main purpose is to validate and check constraints about RDF data makes it less usable to describe RDF subsets.

ShEx was adopted by Wikidata in 2019 to define entity schemas [68].

We could talk more about: - Constraints and validation - Schemas and ontologies - SHACL - Rules and inference

MARS (Multi-Attributed Relational Structures) [50] has been proposed as a logical framework capable to reason about Wikibase data models.

SQID [49] added an inference layer combined with visualization on top of Wikidata.

[45] proposes the use of an extension of MARS to define constraints on wikidata.

Big data processing and graphs

A functional definition of Spark using Haskell has been proposed in [11]. It would be interesting to use that functional specification to prove the correctness of the algorithm proposed in this paper.

Knowledge graphs subsets

In the case of RDF, RDFSlice [46, 47] was proposed as a system that generated RDF data fragments from large endpoints like DBpedia. It defines a subset of SPARQL called sliceSPARQL. A new version, called Torpedo, was proposed in [48].

In the case of Wikidata, WDump³¹ was created as a tool that generates filtered wikidata from dumps. It takes two inputs: a JSON compressed dump and a JSON configuration file that describes the different filters, and generates as output an RDF compressed dump. The tool can be run as a web service locally and is also deployed at <https://tools.wmflabs.org/wdumps>. Its web service allows the user to introduce the different filters filling a form which generates a dump generation request that is added to a queue. It is possible to see the list of previously requested dumps. Once the dump has been generated, it can be uploaded to Zenodo. WDump is divided in two main modules, the backend, which has been implemented in Java using the Wikidata Toolkit library³² and the frontend that has been implemented in Typescript. The use of WDump to generate Wikidata subsets is described in [30] where 4 subsets are created about the topics: politicians, military politicians, UK universities and GeneWiki data. That paper also presents several use case scenarios and discusses some strengths and weaknesses. In this paper, we present a formal definition of WDump in the context of other subset generation approaches like the ShEx-based ones.

The Python library WikidataSets [7] generates Wikidata subsets from specific topics. In the paper the authors generated subsets for the following topics: humans, countries, companies, animal species and films. The tool obtains items following the instances of a topic or subclasses of the topic.

KGTK (Knowledge graph toolkit) [31] presents a tool that works with knowledge graphs by defining a common format called KGTK format based on hypergraphs. It is possible to import

³¹<https://github.com/bennofs/wdumper>

³²<https://github.com/Wikidata/Wikidata-Toolkit>

and export data from different formats like Wikidata or ConceptNet, do several operations over those graphs like: validation, cleaning, graph manipulation (sort, column removal, edge filtering) and graph merging (join, cat) operations. The tool also supports graph querying and analytics operations. Given that KGTK can take as input Wikidata dumps and generate Wikidata dumps as output, it is possible to use KGTK to generate subsets of Wikidata. Further work needs to be done about comparing the performance and usability of KGTK against the approach presented in this paper.

3.10 Conclusions

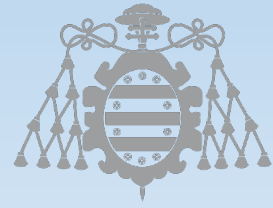
Some ideas:

Should we talk about future work?

- ShEx expressivity
- Discriminators
- Restricts ?? The other day, Andra asked an interesting question...if we can extend a shape adding more properties...could we do the reverse operation, modify a shape removing some properties? We may add a paragraph about this to a discussion section, or talk about it as future work...

3.11 Acknowledgments

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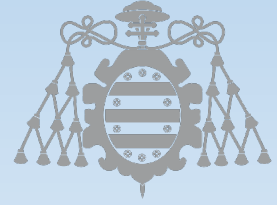
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4. Contribuciones y trabajo futuro

4.1 Contribuciones y resultados conseguidos

Aunque en el artículo se relacionan las principales contribuciones y resultados conseguidos, se describen a continuación con un poco más de detalle y alguna valoración personal relativa al contexto en el que se han producido:

- Se realiza una presentación unificada en la que se definen los grafos RDF, los *property graphs* y los grafos de Wikibase. Las dos primeras definiciones no son nuevas: la definición de grafos RDF es bastante convencional y aparece en numerosos artículos sobre RDF como [24], la definición de *property-graphs* es una adaptación de la definición planteada en [62].
- La definición de Wikibase graphs se considera una aportación de este artículo. En el artículo se presenta una definición formal de lo que se denomina como grafos basados en Wikibase, que son los que se utilizan en Wikidata y otros proyectos basados en la tecnología de Wikibase. La definición está inspirada por el trabajo del artículo [62] en el que se realiza una definición formal de *Property graphs* y el artículo [50] en el que se realiza una definición del formalismo lógico subyacente a los grafos de Wikibase, que denominan MARS *multi-attributed relational structures*.
- Se define un lenguaje para la descripción de *property graphs* denominado PShEx, que es una extensión de ShEx añadiendo restricciones sobre cualificadores para nodos y para relaciones. Esta definición se inspira por un lado en la propia definición de ShEx, definida en [37, 58] y en la propuesta de [62] que añade restricciones inspiradas en SHACL a *property graphs*.
- Se define un lenguaje para la descripción de *Wikibase graphs* denominado WShEx, que es una extensión de ShEx añadiendo restricciones sobre cualificadores sobre relaciones. Esta definición se realiza a partir de la definición de PShEx y permite realizar descripciones del modelo de datos de Wikibase que pueden utilizarse para extraer subconjuntos de Wikidata mediante definiciones en WShEx. Es importante indicar que aunque ShEx puede utilizarse para validar datos en grafos Wikibase mediante esquemas de entidades, en realidad, lo que se valida es la serialización a RDF del modelo de datos de Wikibase. Mediante WShEx se puede describir directamente el modelo de datos de Wikibase tratando los cualificadores como entidades de primer orden.

- Se caracterizan técnicas para extraer subconjuntos de grafos de Wikibase, que permiten comparar las ventajas e inconvenientes de cada una. En concreto, se caracterizan las siguientes técnicas:
 - Subconjuntos generados por entidades (items o propiedades)
 - Subconjuntos generados mediante encaje
 - Subconjuntos generados mediante *slurping*
 - Subconjuntos generados mediante validación a gran escala
- Se define formalmente la técnica de validación en ShEx con *slurping* para WShEx. Esta técnica consiste en recolectar los nodos y tripletas que se encuentran durante el proceso de validación. Aunque los validadores `shex.js`¹ y `PyShEx`² ofrecen una implementación de esta técnica, no existía una definición formal de la misma.
- Se define un algoritmo de validación a gran escala inspirado en el algoritmo Pregel [41]. En el artículo se presenta una descripción formal del algoritmo para el lenguaje WShEx.
- Se lleva a cabo una implementación del algoritmo anterior utilizando la librería Spark GraphX, obteniendo los primeros resultados de validaciones a gran escala que permiten extraer subconjuntos a partir de los nodos validados.

4.2 Líneas futuras de investigación

El trabajo de investigación aquí presentado ha permitido al candidato abrir nuevas líneas de investigación en las cuales todavía no se había trabajado y que se considera que pueden ser prometedoras:

- Finalizar la validación de la implementación en Spark GraphX de los algoritmos aquí presentados. Actualmente, se ha creado un prototipo experimental³ que funciona y ofrece resultados prometedores. Sin embargo, el prototipo trabaja todavía con un subconjunto de ShEx y hay aspectos que todavía están parcialmente implementados.
- Implementar el algoritmo Pregel+ShEx con otras librerías basadas en Prefel como Apache Giraph⁴ que permitan comparar tiempos de respuesta y consumo de recursos.
- Implementar variantes del algoritmo como *ShEx+Slurping* en una misma librería con el fin poder comparar las diferentes técnicas. Actualmente, la generación mediante encaje de grafos está implementada en `WDumper` (Java) y `WDSUB` (Scala), la técnica *ShEx+Slurping* está implementada en `ShEx.js` (Javascript) y `PyShEx` (Python) y el algoritmo ShEx + Pregel está implementado en Scala, con lo que realizar una comparación entre ambos no sería justa al involucrar aspectos asociados a los respectivos lenguajes y entornos.
- Demostrar la corrección de los algoritmos presentados. Actualmente se ha llevado a cabo una implementación que devuelve los resultados esperados pero sería interesante llevar a cabo una demostración más formal de que los resultados generados mediante *ShEx+ Slurping* son equivalentes a los generados mediante *ShEx+Pregel*, por ejemplo.
- Ampliar la expresividad del lenguaje ShEx utilizado en el presente trabajo para incluir negaciones y disyunciones. En la presentación aquí realizada se decidió prescindir de dichos operadores porque su uso no parece necesario para la descripción de subconjuntos y su inclusión complicaba algunas de las definiciones al interactuar con la recursividad. No obstante, una línea de trabajo futuro será analizar en más detalle si pueden incluirse en el lenguaje con una semántica basada en estratificación como se hizo en ShEx [5].
- Dado que los esquemas de entidades existentes utilizan ShEx, sería importante crear una herramienta que permita convertir esquemas ShEx en esquemas WShEx. En principio no

¹<https://github.com/shexjs/shex.js>

²<https://github.com/hsolbrig/PyShEx>

³<https://github.com/weso/sparkwdsb>

⁴<https://giraph.apache.org/>

parece un trabajo complicado desde un punto de vista teórico, dado que sería cuestión de identificar los patrones utilizados en la serialización a RDF de referencias y cualificadores.

- Completar la definición práctica del lenguaje WShEx. Tal y como se ha presentado en el artículo, el lenguaje WShEx tiene una definición simplemente formal, con una implementación que internamente utiliza el analizador sintáctico de ShEx y transforma los esquemas a WShEx. Es necesario desarrollar una gramática para WShEx, decidiendo, por ejemplo cómo distinguir entre referencias y cualificadores. Además, será necesario contemplar cómo representar los tipos de datos complejos utilizados en Wikibase como cantidades, coordenadas geográficas, formas geométricas, tiempos, etc.⁵, así como los rangos⁶.
- La validación mediante Shape Expressions de grandes grafos de conocimiento como Wikidata mediante tecnologías de procesamiento escalables como Apache Spark y Pregel. Esta línea se considera muy prometedora y con grandes aplicaciones, puesto que se desconoce la existencia de validadores que permitan afrontar grafos de conocimiento del tamaño de Wikidata y el algoritmo presentado en el presente trabajo sí lo permite.
- Adaptar y crear herramientas basadas en WShEx para que puedan ser utilizadas por los usuarios de la comunidad Wikibase. A modo de ejemplo, la herramienta Wikishape⁷ podría incluir un editor basado en WShEx que podría por un lado utilizarse para validar entidades, y por otro para crear subconjuntos.
- La definición formal de grafos Wikidata, en un mismo ámbito que los *property graphs* y los grafos RDF, permite la comparación en un mismo marco de dichas tecnologías, facilitando la identificación de las características comunes y diferenciadoras de las mismas. La difusión de este tipo de trabajo sigue la línea de [29] añadiendo un nuevo tipo de grafos de conocimiento que aquí se ha denominado *Wikibase graphs* cuyo modelo de datos es por un lado, una simplificación de los *property graphs* al no admitir cualificadores sobre nodos, pero por otro lado, una generalización de los mismos, al admitir nodos como valores en los cualificadores.

La tabla 4.1 presenta un resumen de las características que se han implementado y las que faltarían por implementarse o que se dejan como trabajo futuro. Se incluye una referencia a los artículos o implementaciones que siguen una determinada técnica. En el caso de que no se haya llevado a cabo la implementación correspondiente se indica mediante el símbolo: Pendiente

4.3 Conclusiones

El trabajo de investigación aquí presentado permite abrir varias líneas de investigación que se desarrollarán en el grupo de investigación.

A corto plazo, el candidato ha sido invitado a liderar el proyecto *21 – Handling Knowledge Graph Subsets*⁸ en el Biohackathon Europe que se celebrará en Barcelona del 8 al 12 de Noviembre de 2021 y en el que se presentarán los primeros resultados de los algoritmos aquí descritos.

Posteriormente, la idea es completar el artículo desarrollado para enviarlo a un congreso o revista especializado. Es posible que incluso se divida el trabajo en 2 o más partes, presentando por un lado las extensiones del lenguaje ShEx para *property graphs* y por otro lado, el trabajo para la creación de subconjuntos de grandes grafos de conocimiento mediante el algoritmo adaptado de Pregel.

Como se puede ver en la tabla 4.1, existen varias celdas que están todavía pendientes de rellenar y que podrían suponer nuevas líneas de trabajo.

El trabajo aquí presentado forma parte de uno de los entregables del proyecto de investigación ANGLIRU descrito en el otro ejercicio, lo cual ha permitido arrancar a trabajar en dicho proyecto,

⁵https://www.mediawiki.org/wiki/Wikibase/DataModel#Datatypes_and_their_Values

⁶https://www.mediawiki.org/wiki/Wikibase/DataModel#Ranks_of_Statements

⁷<https://wikishape.weso.es/>

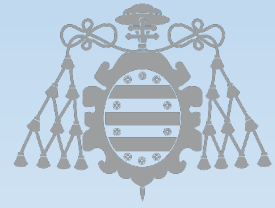
⁸<https://github.com/elixir-europe/biohackathon-projects-2021/tree/main/projects/21>

	Grafos RDF	<i>Property graphs</i>	<i>Wikibase graphs</i>
Definición formal	Realizado Ej.[24]	Realizado [37, 58]	Presente trabajo
Descripción y validación con Shape Expressions	ShEx [5, 58, 65]	PShEx Presente trabajo	WShEx Presente trabajo
Definición formal Entity generated subsets	Pendiente	Pendiente	Presente trabajo
Implementación basada en Entity generated subsets	Pendiente	Pendiente	WDumper
Definición formal Matching generated sub- sets	Pendiente	Pendiente	Presente trabajo
Implementación Matching generated sub- sets	Pendiente	Pendiente	WDumper WDSUB
Definición formal ShEx + Slurping	Pendiente	Pendiente	Presente trabajo
Implementación ShEx+Slurping	shex.js PyShEx	Pendiente	Pendiente
Definición formal ShEx + Pregel	Pendiente	Pendiente	Presente trabajo
Implementación ShEx + Pregel	Pendiente	Pendiente	SparkWDSUB

Cuadro 4.1: Resumen de aspectos realizados anteriormente, desarrollados en el presente trabajo de investigación o pendientes de realizar

ofreciendo unos primeros resultados para el mismo.

El candidato tiene intención de seguir trabajando en las líneas descritas anteriormente, integrando el trabajo desarrollado con el proyecto de investigación ANGLIRU y tratando de contribuir a mejorar la gestión de grafos de conocimiento que, desde una perspectiva más ambiciosa, ayudan a mejorar el conocimiento de la humanidad en general.



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