

Knowledge Graphs

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In this paper we provide a comprehensive introduction to knowledge graphs, which have recently garnered significant attention from both industry and academia in scenarios that require exploiting diverse, dynamic, large-scale collections of data. After some opening remarks, we motivate and contrast various graph-based data models, as well as languages used to query and validate knowledge graphs. We explain how knowledge can be represented and extracted using a combination of deductive and inductive techniques. We conclude with high-level future research directions for knowledge graphs.

CCS Concepts: • **Information systems** → **Graph-based database models**; *Information integration*; • **Computing methodologies** → **Artificial intelligence**;

Additional Key Words and Phrases: knowledge graphs, graph databases, graph query languages, shapes, ontologies, graph algorithms, embeddings, graph neural networks, rule mining

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1 INTRODUCTION

Though the phrase “knowledge graph” has been used in the literature since at least 1972 [118], the modern incarnation of the phrase stems from the 2012 announcement of the Google Knowledge Graph [122], followed by further announcements of knowledge graphs by Airbnb, Amazon, eBay, Facebook, IBM, LinkedIn, Microsoft, Uber, and more besides [57, 95]. The growing industrial uptake of the concept proved difficult for academia to ignore, with more and more scientific literature being published on knowledge graphs in recent years [32, 77, 100, 105, 106, 140, 144].

Knowledge graphs use a graph-based data model to capture knowledge in application scenarios that involve integrating, managing and extracting value from diverse sources of data at large scale [95]. Employing a graph-based abstraction of knowledge has a number of benefits when compared with a relational model or NoSQL alternatives. Graphs provide a concise and intuitive abstraction for a variety of domains, where edges and paths capture different, potentially complex relations between the entities of a domain [6]. Graphs allow maintainers to postpone the definition of a schema, allowing the data to evolve in a more flexible manner [4]. Graph query languages support not only standard relational operators (joins, unions, projections, etc.), but also navigational operators for finding entities connected through arbitrary-length paths [4]. Ontologies [18, 52, 89] and rules [59, 70] can be used to define and reason about the semantics of the terms used in the graph. Scalable frameworks for graph analytics [80, 126, 148] can be leveraged for computing centrality, clustering, summarisation, etc., in order to gain insights about the domain being described. Promising techniques are now emerging for applying machine learning over graphs [140, 145].

1.1 Overview and Novelty

The goal of this tutorial paper is to motivate and give a comprehensive introduction to knowledge graphs, to describe their foundational data models and how they can be queried and validated, and to discuss deductive and inductive ways to make knowledge explicit. Our focus is on introducing key concepts and techniques, rather than specific implementations, optimisations, tools or systems.

A number of related surveys, books, etc., have been published relating to knowledge graphs. In Table 1, we provide an overview of the tertiary literature – surveys, books, tutorials, etc. – relating to knowledge graphs, comparing the topics covered to those specifically covered in this paper. We see that the existing literature tends to focus on particular topics shown. Some of the related literature provides more details on particular topics than this paper; we will often refer to these works for further reading. Unlike these works, our goal as a tutorial paper is to provide a broad and accessible introduction to knowledge graphs. In the final row of the table, we indicate the topics covered in this paper (Ⓒ) and an extended version (Ⓔ) published online [57]. While this paper focuses on the core of knowledge graphs, the extended online version further discusses knowledge graph creation, enrichment, quality assessment, refinement, publication, as well as providing further details of the use of knowledge graphs in practice, their historical background, and formal definitions that complement this paper. We also provide concrete examples relating to the paper in the following repository: <https://github.com/knowledge-graphs-tutorial/examples>.

Our intended audience includes researchers and practitioners who are new to knowledge graphs. As such, we do not assume that readers have specific expertise on knowledge graphs.

Table 1. Related tertiary literature on knowledge graphs; * denotes informal publication (arXiv), ⊙ denotes in-depth discussion, ○ denotes brief discussion, ⊕ denotes discussion in the extended version of this paper [57]

Publication	Year	Type	Models	Querying	Shapes	Context	Ontologies	Entailment	Rules	DLs	Analytics	Embeddings	GNNs	Sym. Learning	Construction	Quality	Refinement	Publication	Enterprise KGs	Open KGs	Applications	History	Definitions	
Pan et al. [97]	2017	Book	○	⊙			○	○			○				⊙						⊙	⊙		
Paulheim [100]	2017	Survey										○			○	○	⊙							
Wang et al. [140]	2017	Survey										⊙		○	○	○	○							
Yan et al. [151]	2018	Survey	○	○					○	⊙	○			○	⊙				⊙	⊙	○			
Gesese et al. [38]	2019	Survey										⊙			⊙						○			
Kazemi et al. [67]	2019	Survey*				○			○			⊙	⊙	⊙	○		○							
Kejriwal [69]	2019	Book													⊙									
Xiao et al. [147]	2019	Survey	○	○		○	○	○							⊙	○						⊙		
Wang and Yang [143]	2019	Survey	○	○			○	○	○		⊙	○	○		⊙	○						○		
Al-Moslmi et al. [2]	2020	Survey													⊙									
Fensel et al. [33]	2020	Book													⊙									
Heist et al. [49]	2020	Survey*					○								⊙	○						⊙		○
Ji et al. [65]	2020	Survey*							⊙			⊙	○		⊙							⊙	○	○
Hogan et al.	2021	Tutorial	⊙	⊙	⊙	⊙	⊙	⊙	⊙	⊙	⊙	⊙	⊙	⊙	⊕	⊕	⊕	⊕	⊕	⊕	⊕	⊕	⊕	⊕

1.2 Terminology

We now establish some core terminology used throughout the paper.

Knowledge graph. The definition of a “knowledge graph” remains contentious [13, 15, 32], where a number of (sometimes conflicting) definitions have emerged, varying from specific technical proposals to more inclusive general proposals.¹ Herein we define a knowledge graph as a *graph of data intended to accumulate and convey knowledge of the real world, whose nodes represent entities of interest and whose edges represent potentially different relations between these entities.* The graph of data (aka *data graph*) conforms to a graph-based data model, which may be a *directed edge-labelled graph*, a *heterogeneous graph*, a *property graph*, etc. (we discuss these models in Section 2).

Knowledge. While many definitions for *knowledge* have been proposed, we refer to what Nonaka and Takeuchi [94] call “*explicit knowledge*”, i.e., something that is known and can be written down. Knowledge may be composed of simple statements, such as “*Santiago is the capital of Chile*”, or quantified statements, such as “*all capitals are cities*”. Simple statements can be accumulated as edges in the data graph. For quantified statements, a more expressive way to represent knowledge – such as *ontologies* or *rules* – is required. *Deductive methods* can then be used to entail and accumulate further knowledge (e.g., “*Santiago is a city*”). Knowledge may be extracted from external sources. Additional knowledge can also be extracted from the knowledge graph itself using *inductive methods*.

Open vs. enterprise knowledge graphs. Knowledge graphs aim to become an ever-evolving shared substrate of knowledge within an organisation or community [95]. Depending on the organisation or community the result may be an *open* or *enterprise* knowledge graph. Open knowledge graphs are published online, making their content accessible for the public good. The most prominent examples – BabelNet [90], DBpedia [76], Freebase [14], Wikidata [138], YAGO [55], etc. – cover many domains, offer multilingual lexicalisations (e.g., names, aliases and descriptions of entities), and are either extracted from sources such as Wikipedia [55, 76, 90], or built by communities of volunteers [14, 138]. Open knowledge graphs have also been published within specific domains, such as media, government, geography, tourism, life sciences, and more besides. Enterprise knowledge

¹A comprehensive discussion of prior definitions can be found in Appendix A of the extended version [57].

graphs are typically internal to a company and applied for commercial use-cases [95]. Prominent industries using enterprise knowledge graphs include Web search, commerce, social networks, finance, among others, where applications include search, recommendations, information extraction, personal agents, advertising, business analytics, risk assessment, automation, and more besides [57].

1.3 Paper Structure

We introduce a running example used throughout the paper, and the paper's structure.

Running example. To keep the discussion accessible, we present concrete examples for a hypothetical knowledge graph relating to tourism in Chile (loosely inspired by, e.g., [66, 79]), aiming to increase tourism in the country and promote new attractions in strategic areas through an online tourist information portal. The knowledge graph itself will eventually describe tourist attractions, cultural events, services, businesses, as well as cities and popular travel routes.

Structure. The remainder of the paper is structured as follows:

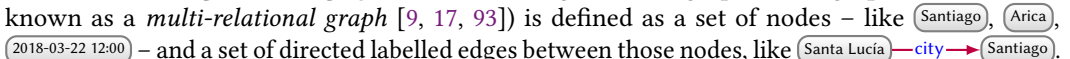

- Section 2** outlines graph data models and the languages used to query and validate them.
- Section 3** presents deductive formalisms by which knowledge can be represented and entailed.
- Section 4** describes inductive techniques by which additional knowledge can be extracted.
- Section 5** concludes with a summary and future research directions for knowledge graphs.

2 DATA GRAPHS

At the foundation of any knowledge graph is the principle of first modelling data as a graph. We now discuss a selection of popular graph-structured data models, languages used to query and validate graphs, as well as representations of context in graphs.

2.1 Models

Graphs offer a flexible way to conceptualise, represent and integrate diverse and incomplete data. We now introduce the graph data models most commonly used in practice [4].

2.1.1 Directed edge-labelled graphs. A directed edge-labelled graph, or del graph for short (also known as a *multi-relational graph* [9, 17, 93]) is defined as a set of nodes – like  – and a set of directed labelled edges between those nodes, like . In knowledge graphs, nodes represent entities (the city Santiago; the hill Santa Lucia; noon on March 22nd, 2018; etc.) and edges represent binary relations between those entities (e.g., Santa Lucia is in the city Santiago). Figure 1 exemplifies how the tourism board could model event data as a del graph. Adding data to such a graph typically involves adding new nodes and edges (with some exceptions discussed later). Representing incomplete information requires simply omitting a particular edge (e.g., the graph does not yet define a start/end date-time for the Food Truck festival).

Modelling data in this way offers more flexibility for integrating new sources of data, compared to the standard relational model, where a schema must be defined upfront and followed at each step. While other structured data models such as trees (XML, JSON, etc.) would offer similar flexibility, graphs do not require organising the data hierarchically (should *venue* be a parent, child, or sibling of *type* for example?). They also allow cycles to be represented and queried (e.g., in Figure 1, note the directed cycle in the routes between Santiago, Arica, and Viña del Mar).

A standard data model based on del graphs is the Resource Description Framework (RDF) [24]. RDF defines three types of nodes: *Internationalised Resource Identifiers* (IRIs), used for globally identifying entities and relations on the Web; *literals*, used to represent strings and other datatype values (integers, dates, etc.); and *blank nodes*, used to denote the existence of an entity.

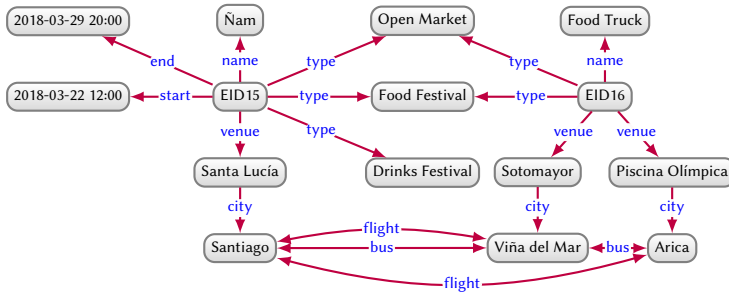


Fig. 1. Directed-edge labelled graph describing events and their venues.



Fig. 2. Data about capitals and countries in a del graph and a heterogeneous graph

2.1.2 *Heterogeneous graphs.* A heterogeneous graph [61, 142, 154] (or *heterogeneous information network* [128, 129]) is a graph where each node and edge is assigned one type. Heterogeneous graphs are thus akin to del graphs – with edge labels corresponding to edge types – but where the type of node forms part of the graph model itself, rather than being expressed as a special relation, as seen in Figure 2. An edge is called *homogeneous* if it is between two nodes of the same type (e.g., *borders*); otherwise it is called *heterogeneous* (e.g., *capital*). Heterogeneous graphs allow for partitioning nodes according to their type, for example, for the purposes of machine learning tasks [61, 142, 154]. However, unlike del graphs, they typically assume a one-to-one relation between nodes and types (notice the node *Santiago* with zero types and *EID15* with multiple types in the del graph of Figure 1).

2.1.3 *Property graphs.* A property graph allows a set of *property–value* pairs and a *label* to be associated with nodes and edges, offering additional flexibility when modelling data [4, 84]. Consider, for example, modelling the airline companies that offer flights. In a del graph, we cannot directly annotate an edge like *Santiago–flight→Arica* with the company, but we could add a new node denoting a flight and connect it with the source, destination, companies, and mode, as shown in Figure 3a. Applying this pattern to a large graph may require significant changes. Conversely, Figure 3b exemplifies a property graph with analogous data, where property–value pairs on edges model companies, property–value pairs on nodes indicate latitudes and longitudes, and node/edge labels indicate the type of node/edge. Though not yet standardised, property graphs are used in popular graph databases, such as Neo4j [4, 84]. While the more intricate model offers greater flexibility in terms of how to encode data as a property graph (e.g., using property graphs, we can continue modelling flights as edges in Figure 3b) potentially leading to a more intuitive representation, these additional details likewise require more intricate query languages, formal semantics, and inductive techniques versus simpler graph models such as del graphs or heterogeneous graphs.

2.1.4 *Graph dataset.* A graph dataset allows for managing several graphs, and consists of a set of *named graphs* and a *default graph*. Each named graph is a pair of a graph ID and a graph. The default graph is a graph without an ID, and is referenced “by default” if a graph ID is not specified. Figure 4 provides an example where events and routes are stored in two named graphs, and the

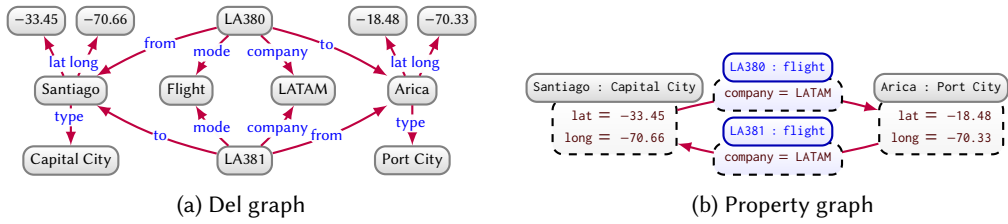


Fig. 3. Flight data in a del graph and a property graph

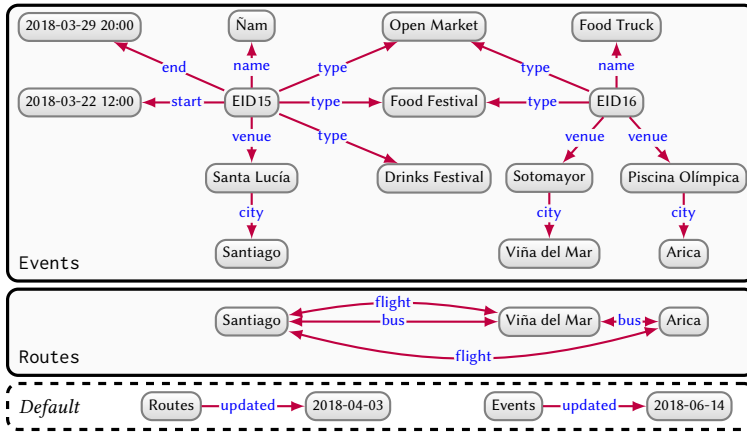


Fig. 4. Graph dataset with two named graphs and a default graph describing events and routes

default graph manages meta-data about the named graphs. Though the example uses del graphs, graph datasets can be generalised to other types of graphs. Graph datasets are useful for managing and querying data from multiple sources [48], where each source can be managed as a separate graph, allowing individual graphs to be queried, updated, removed, etc., as needed.

2.1.5 *Other graph data models.* The graph models presented thus far are the most popular in practice [4]. Other graph data models exist with nodes that may contain individual edges or even nested graphs (aka. *hypernodes*) [6]. Likewise *hypergraphs* allow edges that connect sets rather than pairs of nodes. Nonetheless, data can typically be converted from one model to another; in our view, a knowledge graph can thus adopt any such graph data model. In this paper we discuss del graphs given their relative succinctness, but most discussion extends naturally to other models.

2.1.6 *Graph stores.* A variety of techniques have been proposed for storing and indexing graphs, facilitating the efficient evaluation of queries (as discussed next). Directed-edge labelled graphs can be stored in relational databases either as a single relation of arity three (*triple table*), as a binary relation for each property (*vertical partitioning*), or as *n*-ary relations for entities of a given type (*property tables*) [146]. Custom storage techniques have also been developed for a variety of graph models, providing efficient access for finding nodes, edges and their adjacent elements [6, 84, 146]. A number of systems further allow for distributing graphs over multiple machines based on popular NoSQL stores or custom partitioning schemes [63, 146]. For further details we refer to the book chapter by Janke and Staab [63] and the survey by Wylot et al. [146] dedicated to this topic.

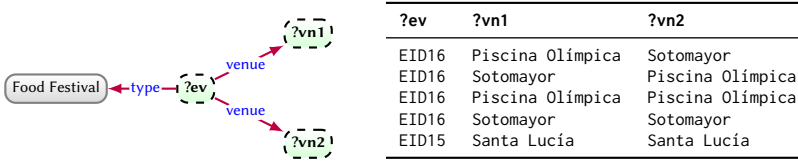


Fig. 5. Graph pattern (left) with mappings generated over the graph of Figure 1 (right)

2.1.7 *Creation.* We have seen how knowledge graphs can be modelled and stored, but how are they created? Creation often involves integrating data from diverse sources, including direct human input; extraction from existing text, markup, legacy file formats, relational databases, other knowledge graphs; etc. [57]. Further discussion on knowledge graph creation, enrichment, quality assessment, refinement and publication is provided in the extended version [57].

2.2 Querying

A number of languages have been proposed for querying graphs [4, 121], including the SPARQL query language for RDF graphs [46]; and Cypher [34], Gremlin [112], and G-CORE [5] for querying property graphs. We now describe some common primitives that underlie these languages [4].

2.2.1 *Graph patterns.* A (basic) graph pattern [4] is a graph just like the data graph being queried, but that may also contain variables. Terms in graph patterns are thus divided into constants, such as **Arica** or **venue**, and variables, which we prefix with question marks, such as **?event** or **?rel**. A graph pattern is then evaluated against the data graph by generating mappings from the variables of the graph pattern to constants in the data graph such that the image of the graph pattern under the mapping (replacing variables with the assigned constants) is contained within the data graph.

Figure 5 shows a graph pattern looking for the venues of Food Festivals, along with the mappings generated by the graph pattern against the data graph of Figure 1. In the latter two mappings, multiple variables are mapped to the same term, which may or may not be desirable depending on the application. Hence a number of semantics have been proposed for evaluating graph patterns [4], amongst which the most important are: *homomorphism-based semantics*, which allows multiple variables to be mapped to the same term such that all mappings shown in Figure 5 would be considered results (this semantics is adopted by SPARQL); and *isomorphism-based semantics*, which requires variables on nodes and/or edges to be mapped to unique terms, thus excluding the latter three mappings of Figure 5 from the results (this semantics is adopted by Cypher for edge variables).

2.2.2 *Complex graph patterns.* A graph pattern transforms an input graph into a table of results (as shown in Figure 5). A *complex graph pattern* [4] then allows the tabular results of one or more graph patterns to be transformed using the relational algebra, as supported in query languages such as SQL, including operators such as projection (π , aka. SELECT), selection (σ , aka. WHERE or FILTER), union (\cup , aka. UNION), difference ($-$, aka. EXCEPT), inner joins (\bowtie , aka. NATURAL JOIN), left outer join ($\bowtie\leftarrow$, aka. LEFT OUTER JOIN or OPTIONAL), anti-join ($\bowtie\triangleright$, aka. NOT EXISTS), etc. Graph query languages such as SPARQL [46] and Cypher [34] then support complex graph patterns.

Figure 6 shows a complex graph pattern looking for food festivals or drinks festivals not held in Santiago, optionally returning their name and start date (where available). We denote projected variables in bold. The complex graph pattern combines the tables of mappings for five basic graph patterns (Q_1, \dots, Q_5) using relational operators ($\cup, \triangleright, \bowtie\leftarrow$) in order to generate the results shown.

Complex graph patterns can give rise to duplicate results; for example, if we project only the variable **?ev**, in Figure 5, then **EID16** appears (alone) as a result four times. Query languages

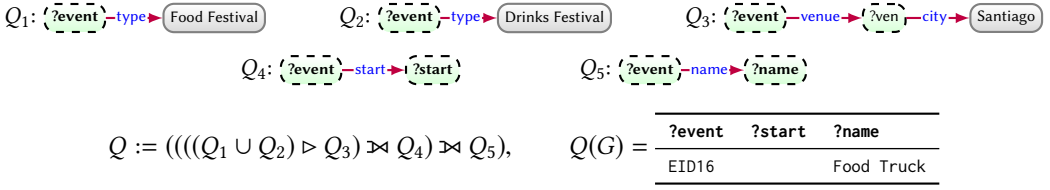


Fig. 6. Complex graph pattern (Q) with mappings generated ($Q(G)$) over the graph of Figure 1 (G)

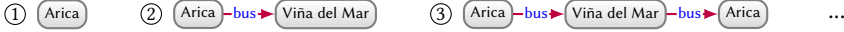


Fig. 7. Navigational graph pattern (left) with mappings generated over the graph of Figure 1 (right)

typically offer two semantics: *bag semantics* preserves duplicates according to the multiplicity of the underlying mappings, while *set semantics* (aka. DISTINCT) removes duplicates from the results.

2.2.3 Navigational graph patterns. A *path expression* r is a regular expression that can be used in a *regular path query* (x, r, y) , where x and y can be variables or constants, in order to match paths of arbitrary length. The base path expression is where r is a constant (an edge label). If r is a path expression, then r^{-} (*inverse*)² and r^* (*Kleene star*: 0-or-more) are also path expressions. If r_1 and r_2 are path expressions, then $r_1 \mid r_2$ (*disjunction*) and $r_1 \cdot r_2$ (*concatenation*) are also path expressions.

Regular path queries can then be evaluated under a number of different semantics. For example, $(\text{Arica}, \text{bus}^*, \{?city\})$ evaluated against the graph of Figure 1 may match the following paths:



In fact, since a cycle is present, an infinite number of paths are potentially matched. For this reason, restricted semantics are often applied, returning only the shortest paths, or paths without repeated nodes or edges (as in the case of Cypher).³ Rather than returning paths, another option is to instead return the (finite) set of pairs of nodes connected by a matching path (as in the case of SPARQL 1.1).

Regular path queries can then be used in graph patterns to express *navigational graph patterns* [4], as shown in Figure 7, which illustrates a query searching for food festivals in cities reachable (recursively) from Arica by bus or flight. Combining regular paths queries with complex graph patterns gives rise to *complex navigational graph patterns* [4], which are supported by SPARQL 1.1.

2.2.4 Other features. Graph query languages may support other features beyond those we have discussed, such as aggregation, complex filters and datatype operators, sub-queries, federated queries, graph updates, entailment regimes, etc. For more information, we refer to the respective query languages (e.g., [5, 46]) and to the survey by Angles et al. [4].

2.3 Validation

While graphs offer a flexible representation for diverse, incomplete data at large-scale, we may wish to validate that our data graph follows a particular structure, or is in some sense “complete”. In Figure 1, for example, we may wish to ensure that all events have at least a name, venue, start

²Some authors distinguish *2-way regular path queries* from regular path queries, where only the former supports inverses.

³Mapping variables to paths requires special treatment [4]. Cypher [34] returns a string that encodes a path, upon which certain functions such as $\text{length}(\cdot)$ can be applied. G-CORE [5], on the other hand, allows for returning paths, and supports additional operators on them, including projecting them as graphs, applying cost functions, and more besides.

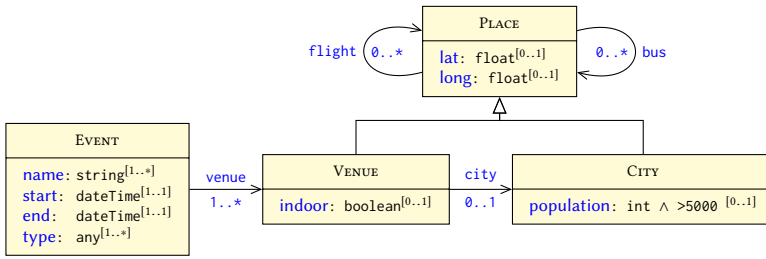


Fig. 8. Example shapes graph depicted as a UML-like diagram

and end date, such that applications using the data – e.g., one notifying users of events – have the minimal information required. One mechanism to facilitate such validation is to use *shapes graphs*.

2.3.1 Shapes graphs. A *shape* [72, 75, 104] targets a set of nodes in a data graph and specifies *constraints* on those nodes. The shape’s target can be specified manually, using a query, etc.

A *shapes graph* is then formed from a set of interrelated shapes. Shapes graphs can be depicted as UML-like class diagrams, where Figure 8 illustrates an example of a shapes graph based on Figure 1, defining constraints on four interrelated shapes. Each shape – denoted with a box like `PLACE`, `EVENT`, etc. – is associated with a set of constraints. Nodes conform to a shape if and only if they satisfy all constraints defined on the shape. Inside each shape box constraints are placed on the number (e.g., `[1..*]` denotes one-to-many, `[1..1]` denotes precisely one, etc.) and types (e.g., `string`, `dateTime`, etc.) of nodes that conforming nodes can relate to with an edge label (e.g., `name`, `start`, etc.). Another option is to place constraints on the number of nodes conforming to a particular shape that the conforming node can relate to with an edge-label (thus generating edges between shapes); for example, `EVENT` $\xrightarrow[\text{venue}]{1..*}$ `VENUE` denotes that conforming nodes for `EVENT` must link to at least one node that conforms to the `VENUE` shape with the edge label `venue`. Shapes can inherit the constraints of parent shapes (denoted with Δ) as per `CITY` and `VENUE` whose parent is `PLACE`.

Boolean combinations of shapes can be defined using conjunction (*AND*), disjunction (*OR*), and negation (*NOT*); for example, we may say that all the values of `venue` should conform to the shape `VENUE AND (NOT CITY)`, making explicit that venues in the data should not be directly given as cities.

When declaring shapes, the data modeller may not know in advance the entire set of properties that some nodes can have. An *open shape* allows the node to have additional properties not specified by the shape, while a *closed shape* does not. For example, if we add the edge `(Santiago) -founder-> (Pedro de Valdivia)` to the graph represented in Figure 1, then `(Santiago)` only conforms to the `CITY` shape if that shape is defined as open (since the shape does not mention `founder`).

2.3.2 Conformance. A node *conforms* to a shape if it satisfies all of the constraints of the shape. The conformance of a node to a shape may depend on the conformance of other nodes to other shapes; for example, the node `(EID15)` conforms to the `EVENT` shape not only based on its local properties, but also based on conformance of `(Santa Lucía)` to `VENUE` and `(Santiago)` to `CITY`. Conformance dependencies may also be recursive, where the conformance of `(Santiago)` to `CITY` requires that it conform to `PLACE`, which requires that `(Viña del Mar)` and `(Arica)` conform to `PLACE`, and so on. Conversely, `(EID16)` does not conform to `EVENT`, as it does not have the `start` and `end` properties required by the shapes graph.

A graph is *valid* with respect to a shapes graph (and its targets) if and only if every node that each shape targets conforms to that shape; for example, if `EVENT` targets `(EID15)` and `(EID16)`, the graph of Figure 1 will not be valid with respect to the shapes graph of Figure 8 (`(EID16)` does not conform to `EVENT`), whereas if `EVENT` targets `(EID15)` only, and no other target is defined, the graph is valid.

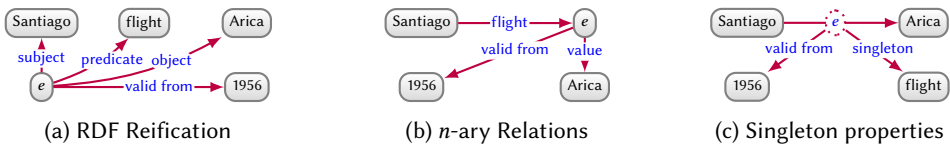


Fig. 9. Three representations of temporal context on an edge in a directed-edge labelled graph

2.3.3 *Other features.* Two shapes languages with such features have been proposed for RDF graphs: *Shape Expressions (ShEx)* [104]; and *SHACL (Shapes Constraint Language)* [72]. These languages also support additional features; for example, SHACL supports constraints expressed using graph queries in the SPARQL language. More details about ShEx and SHACL can be found in the book by Labra Gayo et al. [75]. Similar ideas have been proposed by Angles [3] for property graphs.

2.4 Context

Many (arguably *all*) facts presented in the data graph of Figure 1 can be considered true with respect to a certain *context*. With respect to *temporal context* [23, 44, 114, 115], (Santiago) has existed as a city since 1541, flights from (Arica) to (Santiago) began in 1956, etc. With respect to *provenance* [16, 39, 103], data about (EID15) were taken from – and are thus said to be true with respect to – the Ñam webpage on April 11th, 2020. Other forms of context may also be used and combined, such as to indicate that (Arica) is a Chilean city (*geographic*) since 1883 (*temporal*) per the Treaty of Ancón (*provenance*).

By context we herein refer to the *scope of truth*, and thus talk about the context in which some data are held to be true [42, 81]. The graph of Figure 1 leaves much of its context implicit. However, making context explicit can allow for interpreting the data from different perspectives, such as to understand what held true in 2016, what holds true excluding webpages later found to have spurious data, etc. We now discuss various explicit representations of context.

2.4.1 *Direct representation.* The first way to represent context is to consider it as data no different from other data. For example, the dates for the event (EID15) in Figure 1 can be seen as directly representing an ad hoc form of temporal context [114]. Alternatively, a number of specifications have been proposed to directly represent context in a more standard way, including the *Time Ontology* [23] for temporal context, the *PROV Data Model* [39] for provenance, etc.

2.4.2 *Reification.* Often we may wish to directly define the context of edges themselves; for example, we may wish to state that the edge (Santiago)–flight→(Arica) is valid from 1956. One option is to use *reification*, which allows for describing edges themselves in a graph. Figure 9 presents three forms of reification for modelling temporal context [50]: RDF reification [24], *n*-ary relations [24] and singleton properties [91]. Unlike in a direct representation, *e* is seen as denoting an edge in the graph, not a flight. While *n*-ary relations [24] and singleton properties [91] are more succinct, and *n*-ary relations are more compatible with path expressions, the best choice of reification may depend on the system chosen [50]. Other forms of reification have been proposed in the literature, including, for example, NdFluents [40]. In general, a reified edge does not assert the edge it reifies; for example, we may reify an edge to state that it is no longer valid.

2.4.3 *Higher-arity representation.* We can also use higher-arity representations – that extend the graph model – for encoding context. Taking again the edge (Santiago)–flight→(Arica), Figure 10 illustrates three higher-arity representations of temporal context. First, we can use a named del graph (Figure 10a) to contain the edge and then define the temporal context on the graph name. Second, we can use a property graph (Figure 10b) where the temporal context is defined as an attribute on the edge. Third, we can use *RDF** [47] (Figure 10c): an extension of RDF that allows

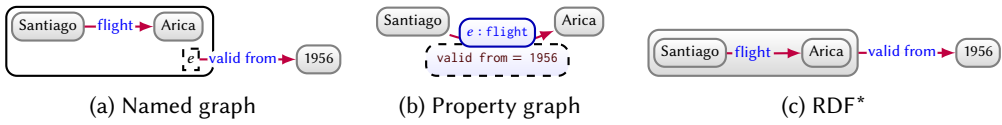


Fig. 10. Three higher-arity representations of temporal context on an edge

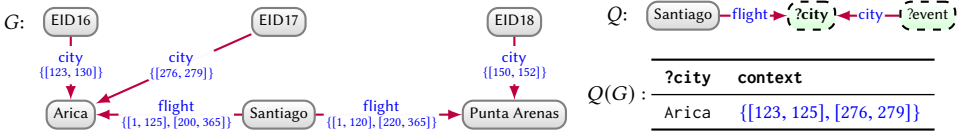


Fig. 11. Example query on a temporally annotated graph

edges to be defined as nodes. The most flexible of the three is the named graph representation, where we can assign context to multiple edges at once by placing them in one named graph, for example, adding more edges valid from 1956 to the named graph of Figure 10a. The least flexible option is RDF*, which, without an edge id, cannot capture different groups of contextual values on an edge; for example, we can add four values to the edge `Chile - president -> M. Bachelet` stating that it was valid from 2006 until 2010 and valid from 2014 until 2018, but we cannot pair the values [50, 115].

2.4.4 Annotations. While the previous alternatives are concerned with representing context, *annotations* allow for defining contexts, which enables automated context-aware processing of data. Some annotations model a particular contextual domain; for example, *Temporal RDF* [44] allows for annotating edges with time intervals, such as `Chile - president -> M. Bachelet` [2006, 2010], while *Fuzzy RDF* [125] allows for annotating edges with a degree of truth such as `Santiago - climate -> Semi-Arid` 0.8, indicating that it is more-or-less true – with a degree of 0.8 – that Santiago has a semi-arid climate.

Other frameworks are domain-independent. *Annotated RDF* [30, 134, 156] allows for representing various forms of context modelled as *semi-rings*: algebraic structures consisting of domain values (e.g., temporal intervals, fuzzy values, etc.) and two main operators to combine domain values: *meet* and *join* (different from the relational algebra join). Figure 11 gives an example where G is annotated with integers (1–365) denoting days of the year. We use an interval notation such that $\{[150, 152]\}$ indicates the set $\{150, 151, 152\}$. Query Q asks for flights from Santiago to cities with events and returns the temporal validity of each answer. To derive these answers, we first apply the *meet operator* – defined here as set intersection – to compute the annotation for which a `flight` and `city` edge match; for example, applying *meet* on $\{[150, 152]\}$ and $\{[1, 120], [220, 365]\}$ for `Punta Arenas` gives the empty time interval $\{\}$, and thus it may be omitted from the results (depending on the semantics chosen). However, for `Arica`, we find two non-empty intersections: $\{[123, 125]\}$ for `EID16` and $\{[276, 279]\}$ for `EID17`. Since we are interested in the city, rather than the event, we combine these two annotations for `Arica` using the *join operator*, returning the annotation in which either result holds true. In our scenario, we define *join* as the union of sets, giving $\{[123, 125], [276, 279]\}$.

2.4.5 Other contextual frameworks. Other frameworks for modelling and reasoning about context in graphs include that of *contextual knowledge repositories* [58], which assign (sub-)graphs to contexts with one or more partially-ordered dimensions (e.g., $2020-03-22 \leq 2020-03 \leq 2020$) allowing to select sub-graphs at different levels of contextual granularity. A similar framework, proposed by Schuetz et al. [120], is based on OLAP-like operations over contextual dimensions.

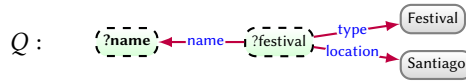


Fig. 12. Graph pattern querying for names of festivals in Santiago

3 DEDUCTIVE KNOWLEDGE

As humans, we can *deduce* more from the data graph of Figure 1 than what the edges explicitly indicate. We may deduce, for example, that the Ñam festival (EID15) will be located in Santiago, that the cities connected by flights must have some airport nearby, etc. Given the data as premises, and some general rules about the world that we may know *a priori*, we can use a deductive process to derive new data, allowing us to know more than what is explicitly given to us by the data.

Machines do not have inherent deductive faculties, but rather need *entailment regimes* to formalise the logical consequence of a given set of premises. Once instructed in this manner, machines can (often) apply deductions with a precision, efficiency, and scale beyond human performance. These deductions may serve a range of applications, such as improving query answering, (deductive) classification, finding inconsistencies, etc. As an example, take the query in Figure 12 asking for *the festivals located in Santiago*. The query returns no results for the graph in Figure 1: there is no node with type (Festival), and nothing has the location (Santiago). However, an answer (Ñam) could be entailed if we stated that x being a Food Festival *entails* that x is a Festival, or that x having venue y in city z *entails* that x has location z . Entailment regimes automate such deductions.

In this section, we discuss ways in which potentially complex entailments can be expressed and automated. Though we could leverage a number of logical frameworks for these purposes – such as First-Order Logic, Datalog, Prolog, Answer Set Programming, etc. – we focus on *ontologies*, which constitute a formal representation of knowledge that, importantly for us, can be represented as a graph; in other words, ontologies can be seen as knowledge graphs with well-defined meaning [32].

3.1 Ontologies

To enable entailment, we must be precise about what the terms we use mean. For example, we have referred to the nodes (EID15) and (EID16) in Figure 1 as “events”. But what if, for example, we wish to define two pairs of start and end dates for (EID16) corresponding to the different venues? Should we rather consider what takes place in each venue as a different event? What if an event has various start and end dates in a single venue: would these be considered one (recurring) event, or many events? These questions are facets of a more general question: *what do we mean by an “event”*? The term “event” may be interpreted in many ways, where the answers are a matter of *convention*.

In computing, an *ontology* is then a concrete, formal representation – a *convention* – on what terms mean within the scope in which they are used (e.g., a given domain). Like all conventions, the usefulness of an ontology depends on how broadly and consistently it is adopted, and how detailed it is. Knowledge graphs that use a shared ontology will be more interoperable. Given that ontologies are formal representations, they can further be used to automate entailment.

Amongst the most popular ontology languages used in practice are the *Web Ontology Language* (OWL) [52], recommended by the W3C and compatible with RDF graphs; and the *Open Biomedical Ontologies Format* (OBOF) [89], used mostly in the biomedical domain. Since OWL is the more widely adopted, we focus on its features, though many similar features are found in both [89]. Before introducing such features, however, we must discuss how graphs are to be *interpreted*.

3.1.1 Interpretations. We as humans may *interpret* the node (Santiago) in the data graph of Figure 1 as referring to the real-world city that is the capital of Chile. We may further *interpret* an edge

$\text{Arica} \xrightarrow{\text{flight}} \text{Santiago}$ as stating that there are flights from the city of Arica to this city. We thus interpret the data graph as another graph – what we here call the *domain graph* – composed of real-world entities connected by real-world relations. The process of interpretation, here, involves *mapping* the nodes and edges in the data graph to nodes and edges of the domain graph.

We can thus abstractly define an *interpretation* [7] of a data graph as the combination of a domain graph and a mapping from the *terms* (nodes and edge-labels) of the data graph to those of the domain graph. The domain graph follows the same model as the data graph. We refer to the nodes of the domain graph as *entities*, and the edges of the domain graph as *relations*. Given a node Santiago in the data graph, we denote the entity it refers to in the domain graph (per a given interpretation) by Santiago . Likewise, for an edge $\text{Arica} \xrightarrow{\text{flight}} \text{Santiago}$, we will denote the relation it refers to by $\text{Arica} \xrightarrow{\text{flight}} \text{Santiago}$. In this abstract notion of an interpretation, we do not require that Santiago or Arica be the real-world cities: an interpretation can have any domain graph and mapping.

3.1.2 Assumptions. Why is this abstract notion of interpretation useful? The distinction between nodes/edges and entities/relations becomes clear when we define the meaning of ontology features and entailment. To illustrate, if we ask whether there is an edge labelled *flight* between Arica and Viña del Mar for the data graph in Figure 1, the answer is *no*. However, if we ask if the entities Arica and Viña del Mar are connected by the relation *flight*, then the answer depends on what *assumptions* we make when interpreting the graph. Under the *Closed World Assumption (CWA)* – which asserts that what is not known is assumed false – without further knowledge the answer is *no*. Conversely, under the *Open World Assumption (OWA)*, it is *possible* for the relation to exist without being described by the graph [7]. Under the *Unique Name Assumption (UNA)*, which states that no two nodes can map to the same entity, we can say that the data graph describes *at least two* flights to Santiago : (since Viña del Mar and Arica must be different entities). Conversely, under the *No Unique Name Assumption (NUNA)*, we can only say that there is *at least one* such flight since Viña del Mar and Arica may be the same entity with two “names” (i.e., two nodes referring to the same entity).

These assumptions define which interpretations are valid, and which interpretations *satisfy* which data graphs. The UNA forbids interpretations that map two nodes to the same entity, while the NUNA does not. Under CWA, an interpretation that contains an edge $x \xrightarrow{p} y$ in its domain graph can only satisfy a data graph from which we can entail $x \xrightarrow{p} y$. Under OWA, an interpretation containing the edge $x \xrightarrow{p} y$ can satisfy a data graph not entailing $x \xrightarrow{p} y$ so long it does not contradict that edge. Ontologies typically adopt the NUNA and OWA, i.e., the most general case, which considers that data may be incomplete, and two nodes may refer to the same entity.

3.1.3 Semantic conditions. Beyond our base assumptions, we can associate certain patterns in the data graph with *semantic conditions* that define which interpretations satisfy it [7]; for example, we can add a semantic condition on a special edge label *subp. of* (subproperty of) to enforce that if our data graph contains the edge $\text{venue} \xrightarrow{\text{subp. of}} \text{location}$, then any edge $x \xrightarrow{\text{venue}} y$ in the domain graph of the interpretation must also have a corresponding edge $x \xrightarrow{\text{location}} y$ in order to satisfy the data graph. These semantic conditions then form the features of an ontology language.

3.1.4 Individuals. In Table 2, we list the main features supported by ontologies for describing *individuals* [52] (aka., entities). First, we can *assert* (binary) relations between individuals using edges such as $\text{Santa Lucía} \xrightarrow{\text{city}} \text{Santiago}$. In the condition column, when we write $x \xrightarrow{y} z$, for example, we refer to the condition that the given relation holds in the interpretation; if so, the interpretation *satisfies* the assertion. We may further assert that two terms refer to the *same* entity, where, e.g., $\text{Región V} \xrightarrow{\text{same as}} \text{Región de Valparaíso}$ states that both refer to the same region; or that two terms refer to *different* entities, where, e.g., $\text{Valparaíso} \xrightarrow{\text{diff. from}} \text{Región de Valparaíso}$ distinguishes the city from the region of the same name. We may also state that a relation does not hold using *negation*.

Table 3. Ontology features for property axioms

Feature	Axiom	Condition (for all x_s, y_s, z_s)	Example
SUBPROPERTY	p -sub. of- q	$x_s \xrightarrow{p} y_s$ implies $x_s \xrightarrow{q} y_s$	venue -sub. of- location
DOMAIN	p -domain- c	$x_s \xrightarrow{p} y_s$ implies x_s type c	venue -domain- Event
RANGE	p -range- c	$x_s \xrightarrow{p} y_s$ implies y_s type c	venue -range- Venue
EQUIVALENCE	p -equiv. p.- q	$x_s \xrightarrow{p} y_s$ iff $x_s \xrightarrow{q} y_s$	start -equiv. p.- begins
INVERSE	p -inv. of- q	$x_s \xrightarrow{p} y_s$ iff $y_s \xrightarrow{q} x_s$	venue -inv. of- hosts
DISJOINT	p -disj. p.- q	not $x_s \xrightarrow{p} y_s$ and $x_s \xrightarrow{q} y_s$	venue -disj. p.- hosts
TRANSITIVE	p -type- Transitive	$x_s \xrightarrow{p} y_s$ and $y_s \xrightarrow{p} z_s$ implies $x_s \xrightarrow{p} z_s$	part of -type- Transitive
SYMMETRIC	p -type- Symmetric	$x_s \xrightarrow{p} y_s$ iff $y_s \xrightarrow{p} x_s$	nearby -type- Symmetric
ASYMMETRIC	p -type- Asymmetric	not $x_s \xrightarrow{p} y_s$ and $y_s \xrightarrow{p} x_s$	capital -type- Asymmetric
REFLEXIVE	p -type- Reflexive	$x_s \xrightarrow{p} x_s$	part of -type- Reflexive
IRREFLEXIVE	p -type- Irreflexive	not $x_s \xrightarrow{p} x_s$	flight -type- Irreflexive
FUNCTIONAL	p -type- Functional	$y_1 \xrightarrow{p} x$ and $y_2 \xrightarrow{p} x$ implies $y_1 = y_2$	population -type- Functional
INV. FUNCTIONAL	p -type- Inv. Functional	$x_1 \xrightarrow{p} y$ and $x_2 \xrightarrow{p} y$ implies $x_1 = x_2$	capital -type- Inv. Functional
KEY	c -key- $\begin{matrix} p_1 \\ \vdots \\ p_n \end{matrix}$	$\begin{matrix} c \\ \vdots \\ c \end{matrix} \xrightarrow{\text{type}} \begin{matrix} x_1 \\ \vdots \\ x_n \end{matrix} \xrightarrow{\begin{matrix} p_1 \\ \vdots \\ p_n \end{matrix}} \begin{matrix} y_1 \\ \vdots \\ y_n \end{matrix}$ implies $x_1 = x_2$	City -key- $\begin{matrix} \text{lat} \\ \text{long} \end{matrix}$
CHAIN	p -chain- $\begin{matrix} q_1 \\ \vdots \\ q_n \end{matrix}$	$x \xrightarrow{q_1} y_1 \xrightarrow{\dots} y_{n-1} \xrightarrow{q_n} z$ implies $x \xrightarrow{p} z$	location -chain- location part of

3.2 Semantics and Entailment

The conditions listed in the previous tables give rise to *entailments*; for example, the definition `nearby-type-Symmetric` and edge `Santiago-nearby-Santiago Airport` entail `Santiago Airport-nearby-Santiago` per the SYMMETRIC condition of Table 3. We now describe how these conditions lead to entailments.

3.2.1 Model-theoretic semantics. Each axiom described by the previous tables, when added to a graph, enforces some condition(s) on the interpretations that *satisfy* the graph. The interpretations that satisfy a graph are called *models* of the graph [7]. If we considered only the base condition of the ASSERTION feature in Table 2, for example, then the models of a graph would be any interpretation such that for every edge $x \rightarrow y \rightarrow z$ in the graph, there exists a relation $x \rightarrow y \rightarrow z$ in the model. Given that there may be other relations in the model (under the OWA), the number of models of any such graph is infinite. Furthermore, given that we can map multiple nodes in the graph to one entity in the model (under the NUNA), any interpretation with (for example) the relation $a \rightarrow a \rightarrow a$ is a model of any graph so long as for every edge $x \rightarrow y \rightarrow z$ in the graph, it holds that $x = y = z = a$ in the interpretation (in other words, the interpretation maps everything to a). As we add axioms with their associated conditions to the graph, we restrict models for the graph; for example, considering a graph with two edges - $x \rightarrow y \rightarrow z$ and `y-type-Irreflexive` - the interpretation with $a \rightarrow a \rightarrow a$, $x = y = \dots = z$ is no longer a model as it breaks the condition for the irreflexive axiom.

Table 4. Ontology features for class axioms and definitions

Feature	Axiom	Condition (for all x_s, y_s, z_s)	Example
SUBCLASS	$c \xrightarrow{\text{subc. of}} d$	$x \text{ type } c \text{ implies } x \text{ type } d$	City $\xrightarrow{\text{subc. of}}$ Place
EQUIVALENCE	$c \xrightarrow{\text{equiv. c.}} d$	$x \text{ type } c \text{ iff } x \text{ type } d$	Human $\xrightarrow{\text{equiv. c.}}$ Person
DISJOINT	$c \xrightarrow{\text{disj. c.}} d$	not $x \text{ type } c \text{ and } x \text{ type } d$	City $\xrightarrow{\text{disj. c.}}$ Region
COMPLEMENT	$c \xrightarrow{\text{comp.}} d$	$x \text{ type } c \text{ iff not } x \text{ type } d$	Dead $\xrightarrow{\text{comp.}}$ Alive
UNION	$c \xrightarrow{\text{union}} \begin{pmatrix} d_1 \\ \vdots \\ d_n \end{pmatrix}$	$x \text{ type } c \text{ iff } x \text{ type } d_1 \text{ or } x \text{ type } d_2 \text{ or } \dots \text{ or } x \text{ type } d_n$	Flight $\xrightarrow{\text{union}}$ $\begin{pmatrix} \text{DomesticFlight} \\ \text{InternationalFlight} \end{pmatrix}$
INTERSECTION	$c \xrightarrow{\text{inter.}} \begin{pmatrix} d_1 \\ \vdots \\ d_n \end{pmatrix}$	$x \text{ type } c \text{ iff } x \text{ type } d_1 \text{ and } x \text{ type } d_2 \text{ and } \dots \text{ and } x \text{ type } d_n$	SelfDrivingTaxi $\xrightarrow{\text{inter.}}$ $\begin{pmatrix} \text{Taxi} \\ \text{SelfDriving} \end{pmatrix}$
ENUMERATION	$c \xrightarrow{\text{one of}} \begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix}$	$x \text{ type } c \text{ iff } x \in \{x_1, \dots, x_n\}$	EUState $\xrightarrow{\text{one of}}$ $\begin{pmatrix} \text{Austria} \\ \vdots \\ \text{Sweden} \end{pmatrix}$
SOME VALUES	$c \xrightarrow{\text{prop some}} \begin{pmatrix} p \\ d \end{pmatrix}$	$x \text{ type } c \text{ iff there exists } a \text{ such that } x \text{ prop } a \text{ and } a \text{ type } d$	EU Citizen $\xrightarrow{\text{prop some}}$ $\begin{pmatrix} \text{nationality} \\ \text{EUState} \end{pmatrix}$
ALL VALUES	$c \xrightarrow{\text{prop all}} \begin{pmatrix} p \\ d \end{pmatrix}$	$x \text{ type } c \text{ iff for all } a \text{ with } x \text{ prop } a \text{ it holds that } a \text{ type } d$	Weightless $\xrightarrow{\text{prop all}}$ $\begin{pmatrix} \text{has part} \\ \text{Weightless} \end{pmatrix}$
HAS VALUE	$c \xrightarrow{\text{prop value}} \begin{pmatrix} p \\ y \end{pmatrix}$	$x \text{ type } c \text{ iff } x \text{ prop } y$	Chilean Citizen $\xrightarrow{\text{prop value}}$ $\begin{pmatrix} \text{nationality} \\ \text{Chile} \end{pmatrix}$
HAS SELF	$c \xrightarrow{\text{prop self}} \begin{pmatrix} p \\ \text{true} \end{pmatrix}$	$x \text{ type } c \text{ iff } x \text{ prop } p$	SelfDriving $\xrightarrow{\text{prop self}}$ $\begin{pmatrix} \text{driver} \\ \text{true} \end{pmatrix}$
CARDINALITY $\star \in \{=, \leq, \geq\}$	$c \xrightarrow{\text{prop } \star} \begin{pmatrix} p \\ n \end{pmatrix}$	$x \text{ type } c \text{ iff } \#\{a \mid x \text{ prop } a\} \star n$	Polyglot $\xrightarrow{\text{prop } \geq}$ $\begin{pmatrix} \text{fluent} \\ 2 \end{pmatrix}$
QUALIFIED CARDINALITY $\star \in \{=, \leq, \geq\}$	$c \xrightarrow{\text{prop class } \star} \begin{pmatrix} p \\ d \\ n \end{pmatrix}$	$x \text{ type } c \text{ iff } \#\{a \mid x \text{ prop } a \text{ and } a \text{ type } d\} \star n$	BinaryStarSystem $\xrightarrow{\text{prop class } =}$ $\begin{pmatrix} \text{body} \\ \text{Star} \\ 2 \end{pmatrix}$

3.2.2 Entailment. We say that one graph *entails* another if and only if any model of the former graph is also a model of the latter graph [7]. Intuitively this means that the latter graph says nothing new over the former graph and thus holds as a logical consequence of the former graph. For example, consider the graph $\text{Santiago} \xrightarrow{\text{type}} \text{City} \xrightarrow{\text{subc. of}} \text{Place}$ and the graph $\text{Santiago} \xrightarrow{\text{type}} \text{Place}$. All models of the latter must have that $\text{Santiago} \text{ type } \text{Place}$, but so must all models of the former, which must have $\text{Santiago} \text{ type } \text{City} \xrightarrow{\text{subc. of}} \text{Place}$ and further must satisfy the condition for SUBCLASS, which requires that $\text{Santiago} \text{ type } \text{Place}$ also hold. Hence we conclude that any model of the former graph must be a model of the latter graph, and thus the former graph entails the latter graph.

3.3 Reasoning

Given two graphs, deciding if the first entails the second – per all of the features in Tables 2–4 – is *undecidable*: no (finite) algorithm for such entailment can exist that halts on all inputs with the correct true/false answer [53]. However, we can provide practical reasoning algorithms for ontologies that (1) halt on any input ontology but may miss entailments, returning false instead of true, (2) always halt with the correct answer but only accept input ontologies with restricted

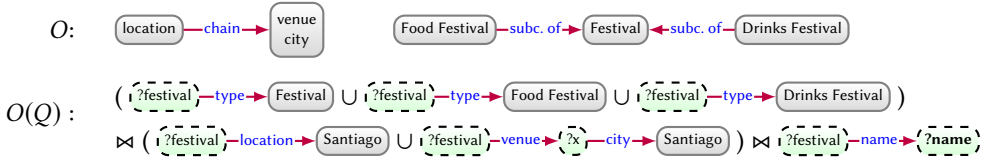


Fig. 13. Query rewriting example for the query Q of Figure 12

features, or (3) only return correct answers for any input ontology but may never halt on certain inputs. Though option (3) has been explored using, e.g., theorem provers for First Order Logic [119], options (1) and (2) are more commonly pursued using rules and/or Description Logics. Option (1) often allows for more efficient and scalable reasoning algorithms and is useful where data are incomplete and having some entailments is valuable. Option (2) may be a better choice in domains – such as medical ontologies – where missing entailments may have undesirable outcomes.

3.3.1 Rules. A straightforward way to implement reasoning is through *inference rules* (or simply *rules*), composed of a *body* (IF) and a *head* (THEN). Both the body and head are given as graph patterns. A rule indicates that if we can replace the variables of the body with terms from the data graph and form a subgraph of a given data graph, then using the same replacement of variables in the head will yield a valid entailment. The head must typically use a subset of the variables appearing in the body to ensure that the conclusion leaves no variables unreplaced. Rules of this form correspond to (positive) Datalog in databases, Horn clauses in logic programming, etc.

Rules can be used to capture entailments under ontological conditions. Here we provide an example of two rules for capturing some of the entailments valid for **SUBCLASS**:

$$\begin{aligned} \widehat{?x} \text{--type--} \widehat{?c} \text{--subc. of--} \widehat{?d} &\Rightarrow \widehat{?x} \text{--type--} \widehat{?d} \\ \widehat{?c} \text{--subc. of--} \widehat{?d} &\Rightarrow \widehat{?c} \text{--subc. of--} \widehat{?e} \end{aligned}$$

A comprehensive set of rules for OWL have been standardised as OWL 2 RL/RDF [87]. These rules are, however, incomplete as such rules cannot fully capture negation (e.g., **COMPLEMENT**), existentials (e.g., **SOME VALUES**), universals (e.g., **ALL VALUES**), or counting (e.g., **CARDINALITY** and **QUALIFIED CARDINALITY**). Other rule languages can, however, support additional such features, including existentials (see, e.g., Datalog[±] [12]), disjunction (see, e.g., Disjunctive Datalog [113]), etc.

Rules can be used for reasoning in a number of ways. *Materialisation* applies rules recursively to a graph, adding entailments back to the graph until nothing new can be added. The materialised graph can then be treated as any other graph; however the materialised graph may become unfeasibly large to manage. Another strategy is to use rules for *query rewriting*, which extends an input query in order to find entailed solutions. Figure 13 provides an example ontology whose rules are used to rewrite the query of Figure 12; if evaluated over the graph of Figure 1, **(Nam)** will be returned as a solution. While not all ontological features can be supported in this manner, query rewriting is sufficient to support complete reasoning over lightweight ontology languages [87].

While rules can be used to (partially) capture ontological entailments, they can also be defined independently of an ontology, capturing entailments for a given domain. In fact, some rules – such as the following – cannot be emulated with the ontology features previously seen, as they do not support ways to infer binary relations from cyclical graph patterns (for computability reasons):

$$\widehat{?x} \text{--flight--} \widehat{?y} \text{--country--} \widehat{?z} \Rightarrow \widehat{?x} \text{--domestic flight--} \widehat{?y}$$

(Note: A red arrow labeled 'country' points from $\widehat{?z}$ back to $\widehat{?x}$ in the original diagram.)

Various languages allow for expressing rules over graphs (possibly alongside ontological definitions) including: Rule Interchange Format (RIF) [70], Semantic Web Rule Language [59], etc.

3.3.2 Description Logics. Description Logics (DLs) hold an important place in the logical formalisation of knowledge graphs: they were initially introduced as a way to formalise the meaning of *frames* [85] and *semantic networks* [107] (which can be seen as predecessors of knowledge graphs) and also heavily influenced OWL. DLs are a family of logics rather than a particular logic. Initially, DLs were restricted fragments of First Order Logic (FOL) that permit decidable reasoning tasks, such as entailment checking [7]. DLs would later be extended with useful features for modelling graph data that go beyond FOL, such as transitive closure, datatypes, etc. Different DLs strike different balances between expressive power and the computational complexity of reasoning.

DLs are based on three types of elements: *individuals*, such as *Santiago*; *classes* (aka *concepts*) such as *City*; and *properties* (aka *roles*) such as *flight*. DLs then allow for making claims, known as *axioms*, about these elements. *Assertional axioms* can be either unary class relations on individuals, such as *City(Santiago)*, or binary property relations on individuals, such as *flight(Santiago,Arica)*. Such axioms form the *Assertional Box* (*A-Box*). DLs further introduce logical symbols to allow for defining *class axioms* (forming the *Terminology Box*, or *T-Box* for short), and *property axioms* (forming the *Role Box*, or *R-Box*); for example, the class axiom $\text{City} \sqsubseteq \text{Place}$ states that the former class is a subclass of the latter one, while the property axiom $\text{flight} \sqsubseteq \text{connectsTo}$ states that the former property is a subproperty of the latter one. DLs also allow for defining classes based on existing terms; for example, we can define a class $\exists \text{nearby.Airport}$ as the class of individuals that have some airport(s) nearby. Noting that the symbol \top is used in DLs to denote the class of all individuals, we can then add a class axiom $\exists \text{flight}.\top \sqsubseteq \exists \text{nearby.Airport}$ to state that individuals with an outgoing flight must have some airport nearby. Noting that the symbol \sqcup can be used in DL to define that a class is the union of other classes, we can further define that $\text{Airport} \sqsubseteq \text{DomesticAirport} \sqcup \text{InternationalAirport}$, i.e., that an airport is either a domestic airport or an international airport (or both).

The similarities between DLs and OWL are not coincidental: the OWL standard was heavily influenced by DLs, where the OWL 2 DL language is a restricted fragment of OWL with decidable entailment. To exemplify one such restriction, with $\text{DomesticAirport} \sqsubseteq =1 \text{ destination} \circ \text{country}.\top$ we can define in DL syntax that domestic airports have flights destined to precisely one country (where $p \circ q$ denotes a chain of properties). However, counting chains is often disallowed in DLs to ensure decidability. For further reading, we refer to the textbook by Baader et al. [7].

Expressive DLs support complex entailments involving existentials, universals, counting, etc. A common strategy for deciding such entailments is to reduce entailment to *satisfiability*, which decides if an ontology is consistent or not.⁵ Thereafter methods such as *tableau* can be used to check satisfiability, cautiously constructing models by completing them along similar lines to the materialisation strategy previously described, but additionally branching models in the case of disjunction, introducing new elements to represent existentials, etc. If any model is successfully “completed”, the process concludes that the original definitions are satisfiable (see, e.g., [88]). Due to their prohibitive computational complexity [87], such reasoning strategies are not typically applied to large-scale data, but may be useful when modelling complex domains.

4 INDUCTIVE KNOWLEDGE

Inductive reasoning generalises patterns from input observations, which are used to generate novel but potentially imprecise predictions. For example, from a graph with geographical and flight information, we may observe that almost all capital cities of countries have international airports serving them, and hence predict that since Santiago is a capital city, it *likely* has an international airport serving it; however, some capitals (e.g., Vaduz) do not have international airports. Predictions may thus have a level of confidence; for example, if we see that 187 of 195

⁵ G entails G' if and only if $G \cup \text{not}(G')$ is not satisfiable.

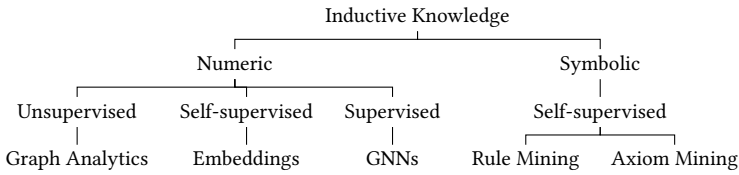


Fig. 14. Conceptual overview of popular inductive techniques for knowledge graphs

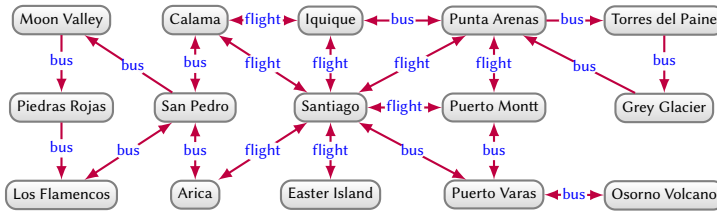


Fig. 15. Data graph representing transport routes in Chile

capitals have an international airport, we may assign a confidence of 0.959 for predictions made with that pattern. We then refer to knowledge acquired inductively as *inductive knowledge*, which includes both the models that encode patterns, and the predictions made by those models.

Inductive knowledge can be acquired from graphs using *supervised* or *unsupervised* methods. Supervised methods learn a function (aka *model*) to map a set of example inputs to their labelled outputs; the model can then be applied to unlabelled inputs. To avoid costly labelling, some supervised methods can generate the input–output pairs automatically from the (unlabelled) input, which are then fed into a supervised process to learn a model; herein we refer to this approach as *self-supervision*. Alternatively, unsupervised processes do not require labelled input–output pairs, but rather apply a predefined function (typically statistical in nature) to map inputs to outputs.

In Figure 14 we provide an overview of the inductive techniques typically applied to knowledge graphs. In the case of unsupervised methods, there is a rich body of work on *graph analytics*, wherein well-known algorithms are used to detect communities or clusters, find central nodes and edges, etc., in a graph. Alternatively, *knowledge graph embeddings* use self-supervision to learn a low-dimensional numerical model of elements of a knowledge graph. The structure of graphs can also be directly leveraged for supervised learning through *graph neural networks*. Finally, *symbolic learning* can learn symbolic models – i.e., logical formulae in the form of rules or axioms – from a graph in a self-supervised manner. We now discuss each of the aforementioned techniques in turn.

4.1 Graph Analytics

Graph analytics is the application of analytical algorithms to (often large) graphs. Such algorithms often analyse the *topology* of the graph, i.e., how nodes and groups thereof are connected. In this section, we provide a brief overview of some popular *graph algorithms* applicable to knowledge graphs, and then discuss *graph processing frameworks* on which such algorithms can be implemented.

4.1.1 Graph algorithms. A wide variety of graph algorithms can be applied for analytical purposes, where we briefly introduce five categories of algorithms that are often used in practice [62].

First, *centrality analysis* aims to identify the most important (“*central*”) nodes or edges of a graph. Specific node centrality measures include *degree*, *betweenness*, *closeness*, *Eigenvector*, *PageRank*, *HITS*, *Katz*, among others. Betweenness centrality can also be applied to edges. A node centrality

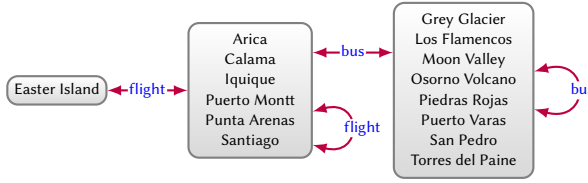


Fig. 16. Example quotient graph summarising the data graph in Figure 15

measure would allow, e.g., to predict the busiest transport hubs in Figure 15, while edge centrality would allow us to find the edges on which many shortest routes depend for predicting traffic.

Second, *community detection* aims to identify sub-graphs that are more densely connected internally than to the rest of the graph (aka. *communities*). Community detection algorithms include *minimum-cut algorithms*, *label propagation*, *Louvain modularity*, etc. Community detection applied to Figure 15 may, for example, detect a community to the left (referring to the north of Chile), to the right (referring to the south of Chile), and perhaps also the centre (referring to cities with airports).

Third, *connectivity analysis* aims to estimate how well-connected and resilient the graph is. Specific techniques include measuring *graph density* or *k-connectivity*, detecting *strongly connected components* and *weakly connected components*, computing *spanning trees* or *minimum cuts*, etc. In the context of Figure 15, such analysis may tell us that routes to Grey Glacier and Piedras Rojas are the most “brittle”, becoming disconnected from the main hubs if one of two bus routes fail.

Fourth, *node similarity* aims to find nodes that are similar to other nodes by virtue of how they are connected within their neighbourhood. Node similarity metrics may be computed using *structural equivalence*, *random walks*, *diffusion kernels*, etc. These methods provide an understanding of what connects nodes, and in what ways they are similar. In Figure 15, such analysis may tell us that Calama and Arica are similar nodes as both have return flights to Santiago and return buses to San Pedro.

Fifth, *graph summarisation* aims to extract high-level structures from a graph, often based on *quotient graphs*, where nodes in the input graph are merged while preserving the edges between the input nodes [21, 57]. Such methods help to provide an overview for a large-scale graph. Figure 16 provides an example of a quotient graph that summarises the graph of Figure 15, such that if there is an edge $s \xrightarrow{p} o$ in the input graph, there is an edge $S \xrightarrow{p} O$ in the quotient graph with $s \in S$ and $o \in O$. In this case, quotient nodes are defined in terms of outgoing edge-labels, where we may detect that they represent islands, cities, and towns/attractions, respectively, from left to right.

Many such techniques have been proposed and studied for simple graphs or directed graphs without edge labels. An open research challenge in the context of knowledge graphs is to adapt such algorithms for graph models such as del graphs, heterogeneous graphs and property graphs [15].

4.1.2 Graph processing frameworks. Various *graph parallel frameworks* have been proposed for large-scale graph processing, including Apache Spark (GraphX) [26, 148], GraphLab [78], Pregel [80], Signal-Collect [126], Shark [149], etc. Computation in these frameworks is iterative, where in each iteration, each node reads messages received through inward edges (and possibly its own previous state), performs a computation, and then sends messages through outward edges using the result.

To illustrate, assume we wish to compute the places that are most (or least) easily reached in the graph of Figure 15. A good way to measure this is using centrality, where we choose PageRank [96], which computes the probability of a tourist that randomly follows the routes shown in the graph being at a particular place after a given number of “hops”. We can implement PageRank on large graphs using a graph parallel framework. In Figure 17, we provide an example of an iteration of PageRank for a sub-graph of Figure 15. The nodes are initialised with a score of $\frac{1}{|V|} = \frac{1}{6}$: a tourist

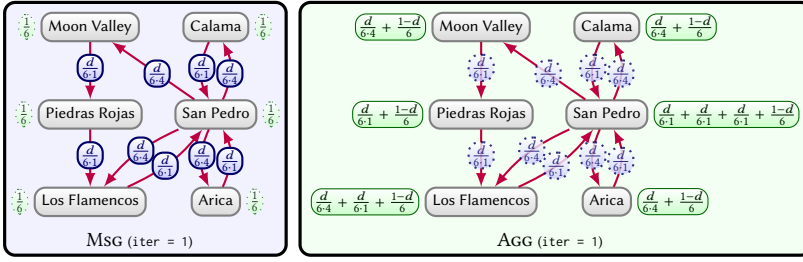


Fig. 17. Example of a graph-parallel iteration of PageRank for a sample sub-graph of Figure 15

is assumed to have an equal chance of starting at any point. In the *message phase* (Msg), each node v passes a score of $\frac{dR_i(v)}{|E(v)|}$ on each of its outgoing edges, where we denote by d a “damping factor” (typically $d = 0.85$) used to ensure convergence, by $R_i(v)$ the score of node v in iteration i (the probability of the tourist being at node v after i hops), and by $|E(v)|$ the number of outgoing edges of v . The aggregation phase (AGG) for v then sums all incoming messages along with its share of the damping factor ($\frac{1-d}{|V|}$) to compute $R_{i+1}(v)$. We then proceed to the message phase of the next iteration, continuing until some termination criterion is reached and results are output.

While the given example is for PageRank, this abstraction is general enough to support a wide variety of (though not all [150]) graph algorithms. An algorithm in this framework consists of the functions to compute message values (Msg), and to accumulate messages (AGG). The framework will then take care of distribution, message passing, fault tolerance, etc.

4.2 Knowledge Graph Embeddings

Machine learning can be used for directly *refining* a knowledge graph [100]; or for *downstream tasks* using the knowledge graph, such as recommendation [155], information extraction [135], question answering [60], query relaxation [139], query approximation [45], etc. However, machine learning techniques typically assume numeric representations (e.g., vectors), distinct from how graphs are usually expressed. So how can graphs be encoded numerically for machine learning?

A first attempt to represent a graph using vectors would be to use a *one-hot encoding*, generating a vector of length $|L| \cdot |V|$ for each node – with $|V|$ the number of nodes in the input graph and $|L|$ the number of edge labels – placing a one at the corresponding index to indicate the existence of the respective edge in the graph, or zero otherwise. Such a representation will, however, typically result in large and sparse vectors, which will be detrimental for most machine learning models.

The main goal of knowledge graph embedding techniques is to create a dense representation of the graph (i.e., *embed* the graph) in a continuous, low-dimensional vector space that can then be used for machine learning tasks. The dimensionality d of the embedding is fixed and typically low (often, e.g., $50 \geq d \geq 1000$). Typically the graph embedding is composed of an *entity embedding* for each node: a vector with d dimensions that we denote by \mathbf{e} ; and a *relation embedding* for each edge label: (typically) a vector with $O(d)$ dimensions that we denote by \mathbf{r} . The overall goal of these vectors is to abstract and preserve latent structures in the graph. There are many ways in which this notion of an embedding can be instantiated. Most commonly, given an edge $\textcircled{s} \text{--} \mathbf{p} \text{--} \textcircled{o}$, a specific embedding approach defines a *scoring function* that accepts \mathbf{e}_s (the entity embedding of node \textcircled{s}), \mathbf{r}_p (the relation embedding of edge label \mathbf{p}) and \mathbf{e}_o (the entity embedding of node \textcircled{o}) and computes the *plausibility* of the edge: how likely it is to be true. Given a data graph, the goal is then to compute the embeddings of dimension d that maximise the plausibility of positive edges (typically edges in the graph) and minimise the plausibility of negative examples (typically edges in the graph with a

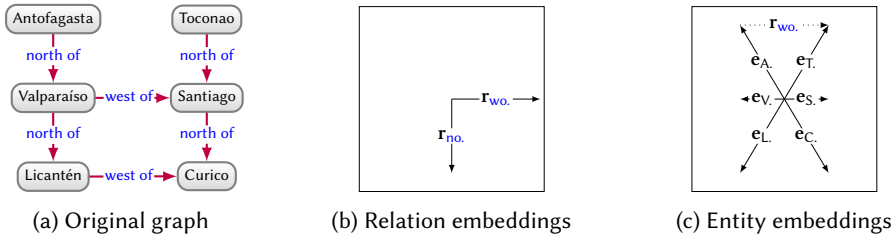


Fig. 18. Toy example of two-dimensional relation and entity embeddings learnt by TransE

node or edge label changed such that they are no longer in the graph) according to the given scoring function. The resulting embeddings can then be seen as models learnt through self-supervision that encode (latent) features of the graph, mapping input edges to output plausibility scores.

Embeddings can then be used for a number of low-level tasks. The plausibility scoring function can be used to assign confidence to edges (possibly extracted from an external source), or to complete edges with missing nodes/edge labels (aka. *link prediction*). Additionally, embeddings will typically assign similar vectors to similar terms, and can thus be used for similarity measures.

A wide range of knowledge graph embedding techniques have been proposed [140], where we summarise the most prominent. First we discuss *translational models* where relations are seen as translating subject entities to object entities. We then describe *tensor decomposition models* that extract latent factors approximating the graph’s structure. Thereafter we discuss *neural models* based on neural networks. Finally, we discuss *language models* based on word embedding techniques.

4.2.1 Translational models. *Translational models* interpret edge labels as transformations from subject nodes (aka the *source* or *head*) to object nodes (aka the *target* or *tail*); for example, in the edge $\text{San Pedro} \xrightarrow{\text{bus}} \text{Moon Valley}$, the edge label *bus* is seen as transforming San Pedro to Moon Valley , and likewise for other *bus* edges. A seminal approach is TransE [17]. Over all positive edges $s \xrightarrow{p} o$, TransE learns vectors e_s , r_p , and e_o aiming to make $e_s + r_p$ as close as possible to e_o . Conversely, if the edge is negative, TransE attempts to learn a representation that keeps $e_s + r_p$ away from e_o . Figure 18 provides a toy example of two-dimensional ($d = 2$) entity and relation embeddings computed by TransE. We keep the orientation of the vectors similar to the original graph for clarity. For any edge $s \xrightarrow{p} o$ in the original graph, adding the vectors $e_s + r_p$ should approximate e_o . In this toy example, the vectors correspond precisely where, for instance, adding the vectors for Licantén (e_L) and *west of* (r_{wo}) gives a vector corresponding to Curico (e_C). We can use these embeddings to predict edges (among other tasks); for example, in order to predict which node in the graph is most likely to be *west of* Antofagasta (A), by computing $e_A + r_{wo}$ we find that the resulting vector (dotted in Figure 18c) is closest to e_T , thus predicting Toconao (T) to be the most *plausible* such node.

Aside from this toy example, TransE can be too simplistic; for example, in Figure 15, *bus* not only transforms San Pedro to Moon Valley , but also to Arica and Calama , where TransE will try to give similar vectors to all target locations, which may not be feasible given other edges. To resolve such issues, many variants of TransE have been investigated, typically using a distinct hyperplane (e.g., TransH [144]) or vector space (e.g., TransR [77], TransD [64]) for each type of relation. Recently, RotatE [130] proposes translational embeddings in complex space, which allows to capture more characteristics of relations, such as direction, symmetry, inversion, antisymmetry, and composition. Embeddings have also been proposed in non-Euclidean space; e.g., MuRP [9] uses relation embeddings that transform entity embeddings in the hyperbolic space of the Poincaré ball mode, whose curvature provides more “space” to separate entities with respect to the dimensionality.

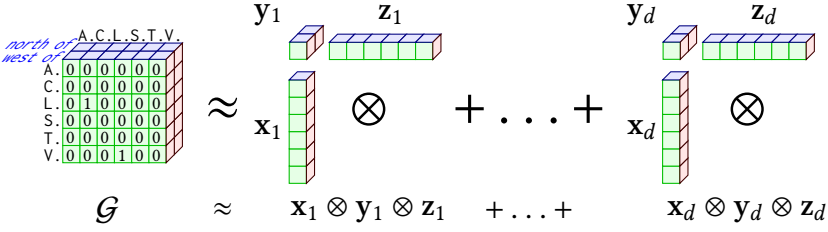


Fig. 19. Abstract illustration of a CP d -rank decomposition of a tensor representing the graph of Figure 18a

4.2.2 Tensor decomposition models. A second approach to derive graph embeddings is to apply methods based on *tensor decomposition*. A *tensor* is a multidimensional numeric field that generalises scalars (0-order tensors), vectors (1-order tensors) and matrices (2-order tensors) towards arbitrary dimension/order. Tensor decomposition involves decomposing a tensor into more “elemental” tensors (e.g., of lower order) from which the original tensor can be recomposed (or approximated) by a fixed sequence of basic operations. These elemental tensors can be seen as capturing *latent factors* in the original tensor. There are many approaches to tensor decomposition, where we will now briefly introduce the main ideas behind *rank decompositions* [108].

Leaving aside graphs, consider an $(a \times b)$ -matrix (i.e., a 2-order tensor) C , where each element $(C)_{ij}$ denotes the average temperature of the i^{th} city of Chile in the j^{th} month of the year. Since Chile is a long, thin country – ranging from subpolar to desert climates – we may decompose C into two vectors representing latent factors – \mathbf{x} (with a elements) giving lower values for cities with lower latitude, and \mathbf{y} (with b elements), giving lower values for months with lower temperatures – such that computing the outer product⁶ of the two vectors approximates C reasonably well: $\mathbf{x} \otimes \mathbf{y} \approx C$. If there exist \mathbf{x} and \mathbf{y} such that $\mathbf{x} \otimes \mathbf{y} = C$, we call C a rank-1 matrix. Otherwise, the rank r of C is the minimum number of rank-1 matrices we need to sum to get precisely C , i.e., $\mathbf{x}_1 \otimes \mathbf{y}_1 + \dots + \mathbf{x}_r \otimes \mathbf{y}_r = C$. In the temperature example, $\mathbf{x}_2 \otimes \mathbf{y}_2$ might correspond to a correction for altitude, $\mathbf{x}_3 \otimes \mathbf{y}_3$ for higher temperature variance further south, etc. A (low) rank decomposition of a matrix then sets a limit d on the rank and computes the vectors $(\mathbf{x}_1, \mathbf{y}_1, \dots, \mathbf{x}_d, \mathbf{y}_d)$ such that $\mathbf{x}_1 \otimes \mathbf{y}_1 + \dots + \mathbf{x}_d \otimes \mathbf{y}_d$ gives the best d -rank approximation of C . Noting that to generate n -order tensors we need to compute the outer product of n vectors, we can generalise this idea towards low rank decomposition of tensors; this method is called Canonical Polyadic (CP) decomposition [51].

To compute knowledge graph embeddings with such techniques, a graph can be encoded as a one-hot 3-order tensor \mathcal{G} with $|V| \times |L| \times |V|$ elements, where the element $(\mathcal{G})_{ijk} = 1$ if the i^{th} node links to the k^{th} node with the j^{th} edge label (otherwise $(\mathcal{G})_{ijk} = 0$). A CP decomposition [51] can compute a sequence of vectors $(\mathbf{x}_1, \mathbf{y}_1, \mathbf{z}_1, \dots, \mathbf{x}_d, \mathbf{y}_d, \mathbf{z}_d)$ such that $\mathbf{x}_1 \otimes \mathbf{y}_1 \otimes \mathbf{z}_1 + \dots + \mathbf{x}_d \otimes \mathbf{y}_d \otimes \mathbf{z}_d \approx \mathcal{G}$, as illustrated in Figure 19. Letting $\mathbf{X}, \mathbf{Y}, \mathbf{Z}$ denote the matrices formed by $[\mathbf{x}_1 \dots \mathbf{x}_d]$, $[\mathbf{y}_1 \dots \mathbf{y}_d]$, $[\mathbf{z}_1 \dots \mathbf{z}_d]$, respectively, with each vector forming a matrix column, we can extract the i^{th} row of \mathbf{Y} as an embedding for the i^{th} relation, and the j^{th} rows of \mathbf{X} and \mathbf{Z} as *two* embeddings for the j^{th} entity. However, knowledge graph embeddings typically aim to assign *one* vector to each entity.

DistMult [152] is a seminal method for computing knowledge graph embeddings based on rank decompositions, where each entity and relation is associated with a vector of dimension d , such that for an edge $\textcircled{s} \text{--} \textcircled{p} \text{--} \textcircled{o}$, a plausibility scoring function $\sum_{i=1}^d (\mathbf{e}_s)_i (\mathbf{r}_p)_i (\mathbf{e}_o)_i$ is defined, where $(\mathbf{e}_s)_i$, $(\mathbf{r}_p)_i$ and $(\mathbf{e}_o)_i$ denote the i^{th} elements of vectors $\mathbf{e}_s, \mathbf{r}_p, \mathbf{e}_o$, respectively. The goal, then, is to learn

⁶The outer product of two (column) vectors \mathbf{x} of length a and \mathbf{y} of length b , denoted $\mathbf{x} \otimes \mathbf{y}$, is defined as $\mathbf{x}\mathbf{y}^T$, yielding an $(a \times b)$ -matrix \mathbf{M} such that $(\mathbf{M})_{ij} = (\mathbf{x})_i \cdot (\mathbf{y})_j$. Analogously, the outer product of k vectors is a k -order tensor.

vectors for each node and edge label that maximise the plausibility of positive edges and minimise the plausibility of negative edges. This approach equates to a CP decomposition of the graph tensor \mathcal{G} , but where entities have one vector that is used twice: $\mathbf{x}_1 \otimes \mathbf{y}_1 \otimes \mathbf{x}_1 + \dots + \mathbf{x}_d \otimes \mathbf{y}_d \otimes \mathbf{x}_d \approx \mathcal{G}$. A weakness of this approach is that per the scoring function, the plausibility of $\textcircled{s} \xrightarrow{p} \textcircled{o}$ will always be equal to that of $\textcircled{o} \xrightarrow{p} \textcircled{s}$; in other words, DistMult does not capture edge direction.

Rather than use a vector as a relation embedding, RESCAL [93] uses a matrix, which allows for combining values from \mathbf{e}_s and \mathbf{e}_o across all dimensions, and thus can capture (e.g.) edge direction. However, RESCAL incurs a higher cost in terms of space and time than DistMult. Recently, ComplEx [132] and HolE [92] both use vectors for relation and entity embeddings, but ComplEx uses complex vectors, while HolE uses a *circular correlation operator* (on reals) [57] in order to capture edge-direction. Simple [68] proposes to compute a standard CP decomposition, averaging terms across X, Y, Z to compute the final plausibility scores. Tucker [10] employs a different type of decomposition – called a Tucker Decomposition [133], which computes a smaller “core” tensor \mathcal{T} and a sequence of three matrices A, B and C , such that $\mathcal{G} \approx \mathcal{T} \otimes A \otimes B \otimes C$ – where entity embeddings are taken from A and C , while relation embeddings are taken from B . Of these approaches, Tucker [10] currently provides state-of-the-art results on standard benchmarks.

4.2.3 Neural models. A number of approaches rather use neural networks in order to learn knowledge graph embeddings with non-linear scoring functions for plausibility.

An early neural model was Semantic Matching Energy (SME) [41], which learns parameters (aka weights: \mathbf{w}, \mathbf{w}') for two functions – $f_w(\mathbf{e}_s, \mathbf{r}_p)$ and $g_{w'}(\mathbf{e}_o, \mathbf{r}_p)$ – such that the dot product of the result of both functions gives the plausibility score. Both linear and bilinear variants of f_w and $g_{w'}$ are proposed. Another early proposal was Neural Tensor Networks (NTN) [123], which maintains a tensor \mathcal{W} of weights and computes plausibility scores by combining the outer product $\mathbf{e}_s \otimes \mathcal{W} \otimes \mathbf{e}_o$ with \mathbf{r}_p and a standard neural layer over \mathbf{e}_s and \mathbf{e}_o . The tensor \mathcal{W} yields a high number of parameters, limiting scalability [140]. Multi Layer Perceptron (MLP) [31] is a simpler model, where $\mathbf{e}_s, \mathbf{r}_p$ and \mathbf{e}_o are concatenated and fed into a hidden layer to compute the plausibility score.

More recent models use convolutional kernels. ConvE [29] generates a matrix from \mathbf{e}_s and \mathbf{r}_p by “wrapping” each vector over several rows and concatenating both matrices, over which (2D) convolutional layers generate the embeddings. A disadvantage is that wrapping vectors imposes an arbitrary two-dimensional structure on the embeddings. HyperER [8] also uses convolutions, but avoids such wrapping by applying a fully connected layer (called the “hypernetwork”) to \mathbf{r}_p in order to generate relation-specific convolutional filters through which the embeddings are generated.

The presented approaches strike different balances in terms of expressivity and the number of parameters that need to be trained. While more expressive models, such as NTN, may better fit more complex plausibility functions over lower dimensional embeddings by using more hidden parameters, simpler models, such as that proposed by Dong et al. [31], and convolutional networks [8, 29] that enable parameter sharing by applying the same (typically small) kernels over different regions of a matrix, require handling fewer parameters overall and are more scalable.

4.2.4 Language models. Embedding techniques were first explored as a way to represent natural language within machine learning frameworks, with word2vec [83] and GloVe [102] being two seminal approaches. Both approaches compute embeddings for words based on large corpora of text such that words used in similar contexts (e.g., “frog”, “toad”) have similar vectors.

Approaches for language embeddings can be applied for graphs. However, while graphs consist of an unordered set of sequences of three terms (i.e., a set of edges), text in natural language consists of arbitrary-length sequences of terms (i.e., sentences of words). Along these lines, RDF2Vec [109] performs biased random walks on the graph and records the paths traversed as “sentences”, which are then fed as input into the word2vec [83] model. An example of such a path extracted from

Figure 15 might be, for example, $\langle \text{San Pedro} \rangle \text{-bus} \rightarrow \langle \text{Calama} \rangle \text{-flight} \rightarrow \langle \text{Iquique} \rangle \text{-flight} \rightarrow \langle \text{Santiago} \rangle$; the paper experiments with 500 paths of length 8 per entity. RDF2Vec also proposes a second mode where sequences are generated for nodes from canonically-labelled sub-trees of which they are a root node, where the paper experiments with sub-trees of depth 1 and 2. Conversely, KGloVe [22] is based on the GloVe model. Much like how the original GloVe model [102] considers words that co-occur frequently in windows of text to be more related, KGloVe uses personalised PageRank to determine the most related nodes to a given node, whose results are then fed into the GloVe model.

4.2.5 Entailment-aware models. The embeddings thus far consider the data graph alone. But what if an ontology or set of rules is provided? One may first consider using constraint rules to refine the predictions made by embeddings. Wang et al. [141] use functional and inverse-functional definitions as constraints (under UNA); for example, if we define that an event can have at most one value for *venue*, the plausibility of edges that would assign multiple venues to an event is lowered.

More recent approaches rather propose joint embeddings that consider both the data graph and rules. KALE [43] computes entity and relation embeddings using a translational model (specifically TransE) that is adapted to further consider rules using *t-norm fuzzy logics*. With reference to Figure 15, consider a simple rule $\langle \tilde{x} \rangle \text{-bus} \rightarrow \langle \tilde{y} \rangle \Rightarrow \langle \tilde{x} \rangle \text{-connects to} \rightarrow \langle \tilde{y} \rangle$. We can use embeddings to assign plausibility scores to new edges, such as $e_1: \langle \text{Piedras Rojas} \rangle \text{-bus} \rightarrow \langle \text{Moon Valley} \rangle$. We can further apply the previous rule to generate a new edge $e_2: \langle \text{Piedras Rojas} \rangle \text{-connects to} \rightarrow \langle \text{Moon Valley} \rangle$ from the predicted edge e_1 . But what plausibility should we assign to e_2 ? Letting p_1 and p_2 be the current plausibility scores of e_1 and e_2 (initialised using the standard embedding), then *t-norm fuzzy logics* suggests that the plausibility be updated as $p_1 p_2 - p_1 + 1$. Embeddings are then trained to jointly assign larger plausibility scores to positive examples of both edges and *ground rules*, i.e., rules with variables replaced by constants from the graph, such as $\langle \text{Arica} \rangle \text{-bus} \rightarrow \langle \text{San Pedro} \rangle \Rightarrow \langle \text{Arica} \rangle \text{-connects to} \rightarrow \langle \text{San Pedro} \rangle$.

Generating ground rules can be costly. An alternative approach, adopted by FSL [28], observes that in the case of a simple rule, such as $\langle \tilde{x} \rangle \text{-bus} \rightarrow \langle \tilde{y} \rangle \Rightarrow \langle \tilde{x} \rangle \text{-connects to} \rightarrow \langle \tilde{y} \rangle$, the relation embedding *bus* should always return a lower plausibility than *connects to*. Thus, for all such rules, FSL proposes to train relation embeddings while avoiding violations of such inequalities. While relatively straightforward, FSL only supports simple rules, while KALE also supports more complex rules.

4.3 Graph Neural Networks

Rather than compute numerical representations for graphs, an alternative is to define custom machine learning architectures for graphs. Most such architectures are based on neural networks [145] given that a neural network is already a directed weighted graph, where nodes serve as artificial neurons, and edges serve as weighted connections (axons). However, the topology of a traditional (fully-connected feed-forward) neural network is quite homogeneous, having sequential layers of fully-connected nodes. Conversely, the topology of a data graph is typically more heterogeneous.

A *graph neural network* (GNN) [117] is a neural network where nodes are connected to their neighbours in the data graph. Unlike embeddings, GNNs support end-to-end supervised learning for specific tasks: given a set of labelled examples, GNNs can be used to classify elements of the graph or the graph itself. GNNs have been used to perform classification over graphs encoding compounds, objects in images, documents, etc.; as well as to predict traffic, build recommender systems, verify software, etc. [145]. Given labelled examples, GNNs can even replace graph algorithms; for example, GNNs have been used to find central nodes in knowledge graphs in a supervised manner [98, 99, 117].

We now introduce two flavours of GNNs: *recursive* and *convolutional*.

4.3.1 Recursive graph neural networks. Recursive graph neural networks (RecGNNs) are the seminal approach to graph neural networks [117, 124]. The approach is conceptually similar to the

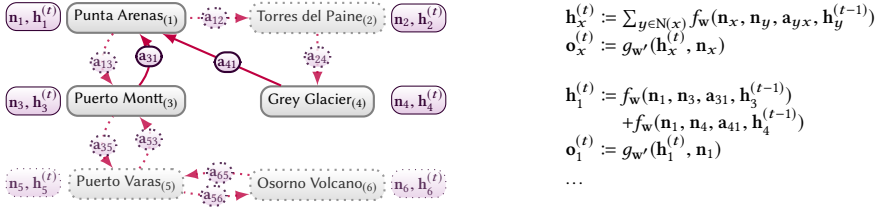


Fig. 20. Illustration of information flowing between neighbours in a RecGNN

abstraction illustrated in Figure 17, where messages are passed between neighbours towards recursively computing some result. However, rather than define the functions used to decide the messages to pass, we rather give labelled examples and let the framework learn the functions.

In a seminal paper, Scarselli et al. [117] proposed what they generically call a graph neural network (GNN), which takes as input a directed graph where nodes and edges are associated with static *feature vectors* that can capture node and edge labels, weights, etc. Each node in the graph also has a *state vector*, which is recursively updated based on information from the node's neighbours – i.e., the feature and state vectors of the neighbouring nodes and edges – using a parametric *transition function*. A parametric *output function* then computes the final output for a node based on its own feature and state vector. These functions are applied recursively up to a fixpoint. Both parametric functions can be learned using neural networks given a partial set of labelled nodes in the graph. The result can thus be seen as a recursive (or even recurrent) neural network architecture. To ensure convergence up to a fixpoint, the functions must be *contractors*, meaning that upon each application, points in the numeric space are brought closer together.

To illustrate, assume that we wish to identify new locations needing tourist information offices. In Figure 20 we illustrate the GNN architecture proposed by Scarselli et al. [117] for a sub-graph of Figure 15, where we highlight the neighbourhood of **Punta Arenas**. In this graph, nodes are annotated with feature vectors (\mathbf{n}_x) and hidden states at step t ($\mathbf{h}_x^{(t)}$), while edges are annotated with feature vectors (\mathbf{a}_{xy}). Feature vectors for nodes may, for example, one-hot encode the type of node (*City*, *Attraction*, etc.), directly encode statistics such as the number of tourists visiting per year, etc. Feature vectors for edges may, for example, one-hot encode the edge label (i.e., the type of transport), directly encode statistics such as the distance or number of tickets sold per year, etc. Hidden states can be randomly initialised. The right-hand side of Figure 20 provides the GNN transition and output functions, where $N(x)$ denotes the neighbouring nodes of x , $f_w(\cdot)$ denotes the transition function with parameters \mathbf{w} , and $g_{w'}(\cdot)$ denotes the output function with parameters \mathbf{w}' . An example is also provided for Punta Arenas ($x = 1$). These functions will be recursively applied until a fixpoint is reached. To train the network, we can label examples of places that already have tourist offices and places that do not have tourist offices. These labels may be taken from the knowledge graph, or may be added manually. The GNN can then learn parameters \mathbf{w} and \mathbf{w}' that give the expected output for the labelled examples, which can subsequently be applied to label other nodes.

4.3.2 Convolutional graph neural networks. Convolutional neural networks (CNNs) have gained a lot of attention, in particular, for machine learning tasks involving images [73]. The core idea in the image setting is to apply small kernels (aka filters) over localised regions of an image using a convolution operator to extract features from that local region. When applied to all local regions, the convolution outputs a feature map of the image. Multiple kernels are typically applied, forming multiple convolutional layers. These kernels can be learnt, given sufficient labelled examples.

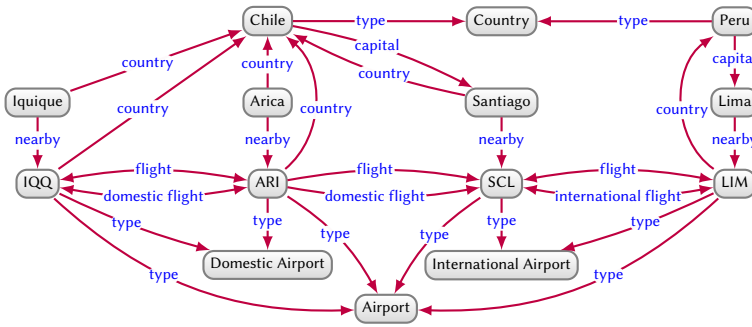


Fig. 21. An incomplete del graph describing flights between airports

Both GNNs and CNNs work over local regions of the input data: GNNs operate over a node and its neighbours in the graph, while (in the case of images) CNNs operate over a pixel and its neighbours in the image. Following this intuition, a number of *convolutional graph neural networks* (ConvGNNs) [145] – aka. *graph convolutional networks* (GCNs) [71] – have been proposed, where the transition function is implemented by means of convolutions. A benefit of CNNs is that the same kernel can be applied over all the regions of an image, but this creates a challenge for ConvGNNs since – unlike in the case of images, where pixels have a predictable number of neighbours – the neighbourhoods of different nodes in a graph can be diverse. Approaches to address these challenges involve working with spectral (e.g. [19, 71]) or spatial (e.g., [86]) representations of graphs that induce a more regular structure from the graph. An alternative is to use an attention mechanism [136] to *learn* the nodes whose features are most important to the current node.

Aside from architectural considerations, there are two main differences between RecGNNs and ConvGNNs. First, RecGNNs aggregate information from neighbours recursively up to a fixpoint, whereas ConvGNNs typically apply a fixed number of convolutional layers. Second, RecGNNs typically use the same function/parameters in uniform steps, while different convolutional layers of a ConvGNN can apply different kernels/weights at each distinct step.

4.4 Symbolic Learning

The supervised techniques discussed thus far learn numerical models that are hard to interpret; for example, taking the graph of Figure 21, knowledge graph embeddings might predict the edge (SCL-flight-ARI) as being highly plausible, but the reason lies implicit in a complex matrix of learnt parameters. Embeddings further suffer from the *out-of-vocabulary* problem, where they are often unable to provide results for inputs involving previously unseen nodes or edge-labels. An alternative is to use *symbolic learning* to learn *hypotheses* in a logical (symbolic) language that “explain” sets of positive and negative edges. Such hypotheses are interpretable; furthermore, they are quantified (e.g., “*all airports are domestic or international*”), partially addressing the out-of-vocabulary issue.

In this section, we discuss two forms of symbolic learning for knowledge graphs: *rule mining* for learning rules, and *axiom mining* for learning other forms of logical axioms.

4.4.1 Rule mining. Rule mining, in the general sense, refers to discovering meaningful patterns in the form of rules from large collections of background knowledge. In the context of knowledge graphs, we assume a set of positive and negative edges as given. The goal of rule mining is to identify new rules that entail a high ratio of positive edges from other positive edges, but entail a low ratio of negative edges from positive edges. The types of rules considered may vary from more simple cases, such as $\langle \tilde{x} \rangle \text{-flight} \rightarrow \langle \tilde{y} \rangle \Rightarrow \langle \tilde{y} \rangle \text{-flight} \rightarrow \langle \tilde{x} \rangle$, to more complex rules, such

as $\langle \bar{x} \rangle \text{--capital--} \langle \bar{y} \rangle \text{--nearby--} \langle \bar{z} \rangle \text{--type--} \langle \text{Airport} \rangle \Rightarrow \langle \bar{z} \rangle \text{--type--} \langle \text{International Airport} \rangle$, indicating that airports near capitals tend to be international airports; or $\langle \bar{x} \rangle \text{--flight--} \langle \bar{y} \rangle \text{--country--} \langle \bar{z} \rangle \Rightarrow \langle \bar{x} \rangle \text{--domestic flight--} \langle \bar{y} \rangle$, indicating that flights within the same country denote domestic flights (as seen in Section 3.3.1).

Per the international airport example, rules are not assumed to hold in all cases, but rather are associated with measures of how well they conform to the positive and negative edges. In more detail, we call the edges entailed by a rule and the set of positive edges (not including the entailed edge itself), the *positive entailments* of that rule. The number of entailments that are positive is called the *support* for the rule, while the ratio of a rule's entailments that are positive is called the *confidence* for the rule [127]. The goal is to find rules with both high support and confidence.

While similar tasks have been explored for relational settings with *Inductive Logic Programming* (ILP) [27], when dealing with an incomplete knowledge graph (under OWA), it is not immediately clear how to define negative edges. A common heuristic is to adopt a *Partial Completeness Assumption* (PCA) [36], which considers the set of positive edges to be those contained in the data graph, and the set of negative examples to be the set of all edges $\langle x \rangle \text{--}p\text{--} \langle y \rangle$ not in the graph but where there exists a node $\langle y \rangle$ such that $\langle x \rangle \text{--}p\text{--} \langle y \rangle$ is in the graph. Taking Figure 21, $\langle \text{SCL} \rangle \text{--flight--} \langle \text{ARI} \rangle$ is a negative edge under PCA (given the presence of $\langle \text{SCL} \rangle \text{--flight--} \langle \text{LIM} \rangle$); conversely, $\langle \text{SCL} \rangle \text{--domestic flight--} \langle \text{ARI} \rangle$ is neither positive nor negative. Under PCA, the support for the rule $\langle \bar{x} \rangle \text{--domestic flight--} \langle \bar{y} \rangle \Rightarrow \langle \bar{y} \rangle \text{--domestic flight--} \langle \bar{x} \rangle$ is then 2 (since it entails $\langle \text{IQQ} \rangle \text{--domestic flight--} \langle \text{ARI} \rangle$ and $\langle \text{ARI} \rangle \text{--domestic flight--} \langle \text{IQQ} \rangle$ in the graph), while the confidence is $\frac{2}{2} = 1$ (noting that $\langle \text{SCL} \rangle \text{--domestic flight--} \langle \text{ARI} \rangle$, though entailed, is neither positive nor negative, and is thus ignored by the measure). The support for the rule $\langle \bar{x} \rangle \text{--flight--} \langle \bar{y} \rangle \Rightarrow \langle \bar{y} \rangle \text{--flight--} \langle \bar{x} \rangle$ is analogously 4, while the confidence is $\frac{4}{5} = 0.8$ (noting that $\langle \text{SCL} \rangle \text{--flight--} \langle \text{ARI} \rangle$ is negative).

An influential rule-mining system for graphs is AMIE [36, 37], which adopts the PCA measure of confidence, and builds rules in a top-down fashion [127] starting with rule heads of the form $\Rightarrow \langle \bar{x} \rangle \text{--country--} \langle \bar{y} \rangle$ for each edge label. For each such rule head, three types of *refinements* are considered, which add an edge with: (1) one existing variable and one fresh variable; for example, refining the aforementioned rule head might give: $\langle \bar{z} \rangle \text{--flight--} \langle \bar{x} \rangle \Rightarrow \langle \bar{x} \rangle \text{--country--} \langle \bar{y} \rangle$; (2) an existing variable and a node from the graph; for example, refining the above rule might give: $\langle \text{Domestic Airport} \rangle \text{--type--} \langle \bar{z} \rangle \text{--flight--} \langle \bar{x} \rangle \Rightarrow \langle \bar{x} \rangle \text{--country--} \langle \bar{y} \rangle$; (3) two existing variables; for example, refining the above rule might give: $\langle \text{Domestic Airport} \rangle \text{--type--} \langle \bar{z} \rangle \text{--flight--} \langle \bar{x} \rangle \langle \bar{y} \rangle \Rightarrow \langle \bar{x} \rangle \text{--country--} \langle \bar{y} \rangle$. Combining

refinements gives rise to an exponential search space that can be pruned. First, if a rule does not meet the support threshold, its refinements need not be explored as refinements (1–3) reduce support. Second, only rules up to fixed size are considered. Third, refinement (3) is applied until a rule is *closed*, meaning that each variable appears in at least two edges of the rule (including the head); the previous rules produced by refinements (1) and (2) are not closed since $\langle \bar{y} \rangle$ appears once.

Later works have built on these techniques for mining rules from knowledge graphs. Gad-Elrab et al. [35] propose a method to learn non-monotonic rules – rules with negated edges in the body – in order to capture exceptions to base rules; for example, the approach may learn a rule $\langle \text{International Airport} \rangle \text{--} \neg \text{type--} \langle \bar{z} \rangle \text{--flight--} \langle \bar{x} \rangle \langle \bar{y} \rangle \Rightarrow \langle \bar{x} \rangle \text{--country--} \langle \bar{y} \rangle$, indicating that flights are within the

same country *except* when the (departure) airport is international (the exception is dotted and \neg is used to negate an edge). The RuLES system [54] also learns non-monotonic rules, and extends the confidence measure to consider the plausibility scores of knowledge graph embeddings for entailed edges not appearing in the graph. In lieu of PCA, the CARL system [101] uses knowledge of the cardinalities of relations to find negative edges, while d'Amato et al. [25] use ontologically-entailed negative edges for measuring the confidence of rules generated by an evolutionary algorithm.

Another line of research is on *differentiable rule mining* [111, 116, 153], which enables end-to-end learning of rules by using matrix multiplication to encode joins in rule bodies. First consider

one-hot encoding edges with label p by an *adjacency matrix* A_p of size $|V| \times |V|$. Now given $(\tilde{x}) \text{--domestic flight--} (\tilde{y}) \text{--country--} (\tilde{z}) \Rightarrow (\tilde{x}) \text{--country--} (\tilde{z})$, we can denote the body by the matrix multiplication $A_{df} A_c$, which gives an adjacency matrix representing entailed **country** edges, where we expect the 1's in $A_{df} A_c$ to be covered by the head's adjacency matrix A_c . Given adjacency matrices for all edge labels, we are left to learn confidence scores for individual rules, and to learn rules (of varying length) with a threshold confidence. Along these lines, NeuralLP [153] uses an *attention mechanism* to find variable-length sequences of edge labels for path-like rules of the form $(\tilde{x}) \text{--} p_1 \text{--} (\tilde{y}_1) \text{--} p_2 \text{--} \dots \text{--} p_n \text{--} (\tilde{y}_n) \text{--} p_{n+1} \text{--} (\tilde{z}) \Rightarrow (\tilde{x}) \text{--} p \text{--} (\tilde{z})$, for which confidences are likewise learnt. DRUM [116] also learns path-like rules, where, observing that some edge labels are more/less likely to follow others – for example, **flight** should not be followed by **capital** in the graph of Figure 15 as the join will be empty – the system uses bidirectional recurrent neural networks (a technique for learning over sequential data) to learn sequences of relations for rules. These differentiable rule mining techniques are, however, currently limited to learning path-like rules.

4.4.2 Axiom mining. Aside from rules, more general forms of axioms – expressed in logical languages such as DLs (see Section 3.3.2) – can be mined from a knowledge graph. We can divide these approaches into two categories: those mining specific axioms and more general axioms.

Among works mining specific types of axioms, disjointness axioms are a popular target; for example, the disjointness axiom $\text{DomesticAirport} \sqcap \text{InternationalAirport} \equiv \perp$ states that the intersection of the two classes is equivalent to the empty class, i.e., no individual can be instances of both classes. Völker et al. [137] extract disjointness axioms based on (negative) *association rule mining* [1], which finds pairs of classes where each has many instances in the knowledge graph but there are relatively few (or no) instances of both classes. Töpfer et al. [131] rather extract disjointness for pairs of classes that have a cosine similarity – computed over the nodes and edge-labels associated with a given class – below a fixed threshold. Rizzo et al. [110] propose an approach that can further capture disjointness constraints between class *descriptions* (e.g., *city without an airport nearby* is disjoint from *city that is the capital of a country*) using a *terminological cluster tree* that first extracts class descriptions from clusters of similar nodes, and then identifies disjoint pairs of class descriptions.

Other systems propose methods to learn more general axioms. A prominent such system is DL-Learner [20], which is based on algorithms for *class learning* (aka *concept learning*), whereby given a set of positive nodes and negative nodes, the goal is to find a logical class description that divides the positive and negative sets. For example, given $\{\text{Iquique}, \text{Arica}\}$ as the positive set and $\{\text{Santiago}\}$ as the negative set, we may learn a (DL) class description $\exists \text{nearby.Airport} \sqcap \neg(\exists \text{capital} \top)$, denoting entities near to an airport that are not capitals, of which all positive nodes are instances and no negative nodes are instances. Like AMIE, such class descriptions are discovered using a refinement operator used to move from more general classes to more specific classes (and vice-versa), a confidence scoring function, and a search strategy. The system further supports learning more general axioms through a scoring function that determines what ratio of edges that would be entailed were the axiom true are indeed found in the graph; for example, to score the axiom $\exists \text{flight} \text{--DomesticAirport} \sqsubseteq \text{InternationalAirport}$ over Figure 21, we can use a graph query to count how many nodes have incoming flights from a domestic airport (there are 3), and how many nodes have incoming flights from a domestic airport *and* are international airports (there is 1), where the greater the difference between both counts, the weaker the evidence for the axiom.

5 SUMMARY AND CONCLUSION

We have given a comprehensive introduction to knowledge graphs. Defining a knowledge graph as *a graph of data intended to accumulate and convey knowledge of the real world, whose nodes represent entities of interest and whose edges represent potentially different relations between these entities*, we

have discussed models by which data can be structured, queried and validated as graphs; we also discussed techniques for leveraging deductive and inductive knowledge over graphs.

Knowledge graphs serve as a common substrate of knowledge within an organisation or community, enabling the representation, accumulation, curation, and dissemination of knowledge over time [95]. In this role, knowledge graphs have been applied for diverse use-cases, ranging from commercial applications – involving semantic search, user recommendations, conversational agents, targeted advertising, transport automation, etc. – to open knowledge graphs made available for the public good [57]. General trends include: (1) the use of knowledge graphs to integrate and leverage data from diverse sources at large scale; and (2) the combination of deductive (rules, ontologies, etc.) and inductive techniques (machine learning, analytics, etc.) to represent and accumulate knowledge.

Future directions. Research on knowledge graphs can become a confluence of techniques from different areas with the common objective of maximising the knowledge – and thus value – that can be distilled from diverse sources at large scale using a graph-based data abstraction [56].

Particularly interesting topics for knowledge graphs arise from the intersections of areas. In the intersection of data graphs and deductive knowledge, we emphasise emerging topics such as *formal semantics for property graphs*, with languages that can take into account the meaning of labels and property–value pairs on nodes and edges [74]; and *reasoning and querying over contextual data*, in order to derive conclusions and results valid in a particular setting [58, 120, 156]. In the intersection of data graphs and inductive knowledge, we highlight topics such as *similarity-based query relaxation*, allowing to find approximate answers to exact queries based on numerical representations (e.g., embeddings) [139]; *shape induction*, in order to extract and formalise inherent patterns in the knowledge graph as constraints [82]; and *contextual knowledge graph embeddings* that provide numeric representations of nodes and edges that vary with time, place, etc. [67, 154]. Finally, in the intersection of deductive and inductive knowledge, we mention the topics of *entailment-aware knowledge graph embeddings* [28, 43], that incorporate rules and/or ontologies when computing plausibility; *expressive graph neural networks* proven capable of complex classification analogous to expressive ontology languages [11]; as well as further advances on *rule and axiom mining*, allowing to extract symbolic, deductive representations from the knowledge graphs [20, 37].

Aside from specific topics, more general challenges for knowledge graphs include *scalability*, particularly for deductive and inductive reasoning; *quality*, not only in terms of data, but also the models induced from knowledge graphs; *diversity*, such as managing contextual or multi-modal data; *dynamicity*, considering temporal or streaming data; and finally *usability*, which is key to increasing adoption. Though techniques are continuously being proposed to address precisely these challenges, they are unlikely to ever be completely “solved”; rather they serve as dimensions along which knowledge graphs, and their techniques, tools, etc., will continue to mature.

Extended version and online material: We refer to the extended version [57] for discussion of further topics relating to knowledge graphs and formal definitions. We provide concrete examples relating to the paper in the following repository: <https://github.com/knowledge-graphs-tutorial/examples>.

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