

Inverting knowledge graphs back to raw data

How can we leverage the rules we use to construct knowledge graphs to do the inverse?

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Contents

Contents	iii
1 Introduction	1
1.1 Thesis outline	2
2 Related work	4
2.1 Semantic Web	4
2.2 RDF	4
2.2.1 Turtle	5
2.3 SPARQL	7
2.4 Mapping languages	7
2.4.1 R2RML	8
2.4.2 RML	9
3 Implementation	10
3.1 General structure	10
3.1.1 Loading the mapping rules	10
3.2 Constructing the schema	12
4 Evaluation	13
4.1 RML test cases	13
5 Conclusion	14

Chapter 1

Introduction

The earliest academic definition of a knowledge graph can be found in a 1974 article as

A mathematical structure with vertices as knowledge units connected by edges that represent the prerequisite relation (Marchi and Miguel, 1974; Bergman, 2019)

The idea of expressing knowledge in a graph structure predates even this definition, with the concept of semantic networks (Richens, 1956). However, the term knowledge graph only became well-known after Google announced they were using a knowledge graph to enhance their search engine in 2012 (Singhal, 2012). Knowledge graphs are used to make search engines, chatbots, question-answering systems, etc more intelligent by injecting knowledge into them (Ji et al., 2022).

A knowledge graph consists of many connected nodes, where each node is either an entity or a literal. These nodes are connected by edges, where each edge defines a relation between two nodes. RDF is a framework often used to represent knowledge graphs, it uses subject-predicate-object triples to represent the nodes and their edges. Every node is either an URI, a blank node, or a literal. The edges are URIs. A triple representing the fact that the entity John Doe has the first name John would look like this: `http://example.com/JohnDoe http://schema.org/givenName "John"`. Often the predicates are chosen from an ontology/vocabulary, such as schema.org or FOAF. This allows for more interoperability between knowledge graphs, as the same predicates are used to represent the same concepts.

These knowledge graphs are constructed by extracting information from various sources, both unstructured sources such as text (using natural language processing) and (semi-)structured sources such as databases, CSV, XML, JSON, RDF (using mapping languages). Many mapping languages exist, differing in the way of defining the rules and the target source file format. Some mapping languages use the turtle syntax, while others provide their custom syntax, and others repurpose existing languages like SPARQL or ShEx. (Van Assche et al., 2023). Some languages are specific to a single source format, such as R2RML(turtle format) (Das et al., 2012) for relational databases, XSPARQL(SPARQL format) (Bischof et al., 2012) for XML. Others can process multiple formats, such as RML (turtle) (Dimou et al., 2014), D-REPR (YAML), xR2RML (turtle), etc. These can handle mapping from multiple sources in different formats.

To achieve this these mapping languages use a declarative approach, where the user specifies the mapping rules, and the implementation of the mapping language takes care of the actual mapping. Two ways of mapping exist, materialization and virtualization. Materialization constructs the knowledge graph as a file, which can be loaded into a triple store. Virtualization does not generate the knowledge graph as a file, but instead exposes a virtual knowledge graph, which can be queried as if it were a real knowledge graph. (Calvanese et al., 2017).

Creating these mapping rules is often done by hand. Some tools make creating these mappings easier, like RMLEditor (Heyvaert et al., 2018b) which exposes a visual editor, and YARRRML (Heyvaert et al., 2018a) which allows users to create rules in the user-friendly YAML which are then compiled to RML rules. Alternatively, tools are starting to be created for the automatic generation of mapping rules from e.g. SHACL.

Retrieving data from a knowledge graph, for consumption by other programs, is done by querying the knowledge graph using SPARQL (Seaborne and Prud'hommeaux, 2008) for tabular data and XSPARQL (Bischof et al., 2012) or XSLT for XML. XSPARQL is the only language that can both map[/lift] and query[/lower], but the syntax for mapping and querying differs, so it could be argued that XSPARQL is two languages.

We can not convert the knowledge graph back to the original data format using the same rules we created it with. As such any changes we make to the data are hard to propagate back to the original data. We can not update, expand, or improve the original data using e.g. knowledge graph refining. Nor can we apply changes to a virtual knowledge graph to change the original data.

In our work, we seek to answer the question: *How can we extend an existing system like RML or create a new system to construct raw data from knowledge graphs?* We choose to extend the Morph-KGC implementation (Arenas-Guerrero et al., 2022) of RML (Dimou et al., 2014) as RML's end-to-end (from file to knowledge graph) characteristics make it a good candidate for this task. To answer the main research question we need to answer the following sub-questions:

RQ1 How can we construct the schema of the original data from the mapping rules?

RQ2 How can we populate the schema with data from the knowledge graph?

1.1 Thesis outline

This thesis aims to explore the possibility of inverting knowledge graphs back to their original data format using RML mapping rules. To achieve this we will first look at the current state of the art in chapter 2. We will take a closer look at the technologies used like RDF, SPARQL, and RML. We will also look at the current state of the art for inverting knowledge graphs. In chapter 3 we will look at our implementation of the inversion algorithm. We will look at the algorithm itself, and the implementation details. In chapter 4 we will evaluate our implementation using various benchmarks. For basic testing, we use a subset of the rml test cases, which are designed to test the conformance of tools to the RML specification. For more advanced testing we will use various benchmarks simulating real-life use cases like LUBM4OBDA, GTFS-Madrid-Bench, and SDM-Genomic-dataset. Finally in chapter 5 we will conclude this thesis, and look at possible future

work.

Chapter 2

Related work

Introduction text providing an overview of the related work

2.1 Semantic Web

Tim Berners-Lee envisioned a version of the web that would also be understandable by machines, and thus the semantic web was born. It is not designed as a separate entity to the web, but instead as an extension, mostly hidden for normal humans. It is designed with mostly existing technologies like XML(including HTML, being a superset of it), URI and RDF. Even ontologies, a key component of the semantic web, are not a new concept but rather co-opted from the field of philosophy. (Berners-Lee et al., 2001)

2.2 RDF

RDF was originally designed as a data model for metadata but has been extended to be a general-purpose framework for graph data. RDF is a directed graph, where the nodes represent entities, and the edges represent relations between these entities. This graph is built up from triples, which connect a subject and an object using a predicate as shown in figure 2.1.

The subject must always be an entity, which can either be represented by an URI or be a blank node. The predicate must be an URI, and the object can be either an URI, a blank node, or a literal. (Manola and Miller, 2004)

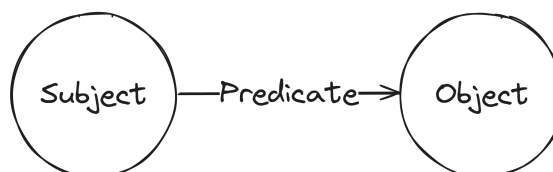


Figure 2.1: An RDF triple

Subject	Predicate	Object
<code>http://example.com/De_Nayer</code>	<code>https://schema.org/location</code>	<code>http://example.com/Sint_Katelijne_Waver</code>
<code>http://example.com/r0785695</code>	<code>https://schema.org/givenName</code>	<code>"Tijs"</code>

Figure 2.2: Example of RDF triples

Subject	Predicate	Object
<code>ex:student/r0785695</code>	<code>schema:address</code>	<code>_:addr0785695</code>
<code>_:addr0785695</code>	<code>schema:postalCode</code>	<code>"2800"^^xsd:integer</code>
<code>_:addr0785695</code>	<code>schema:streetAddress</code>	<code>"Gentsesteenweg XXXX"@nl</code>

Figure 2.3: Example of a blank node and prefix notation

An URI is a unique identifier for a resource on the web. Unlike a normal URL, it does not have to point to a network location, but can also be used to identify a person, a location, a concept, etc. (Manola and Miller, 2004). In RDF the URI is purely used for identifying resources. As such, unlike in HTML where certain conventions are expected, there are no conventions for URIs in RDF. An example of this can be seen in figure 2.2, the example subjects share the same domain but this does not imply that they are closely related, or even related at all. URIs are extended to IRIs to allow for a wider range of characters. Except for allowing Unicode characters, IRIs are identical to URIs so little distinction is made between the two in this thesis.

A blank node is a node that is not identified by a URI. It is used to represent an anonymous resource that can't be or has no reason to be uniquely identified. For example, the address of student `r0785695` in figure 2.3 is only pertinent to the student and thus does not need to be uniquely identified. A blank node is serialized as `_:name`, where `name` is a unique identifier for the blank node. This identifier is unique within the document, and thus can't be used to refer to the blank node from outside the document. (Manola and Miller, 2004)

A literal is a value, e.g. a string, integer, or date. This value can be typed, e.g. a string can be typed as a date, or untyped. A string can also have a language tag, which is used to indicate the language of the literal.

RDF is only a framework, and as such does not define any serialization syntax. There are however a few common serialization standards for example RDF/XML, Turtle, N-Triples, and JSON-LD.

2.2.1 Turtle

Turtle, or Terse RDF Triple Language, is a human-readable serialization format for RDF. It is the most used serialization format for RDF, and is used in many tools and specifications. In its simplest form turtle consists of triple statements, sequences of subject-predicate-object separated by spaces and terminated by a dot. An example of this can be seen in listing 2.1. This is very verbose, but Turtle offers many features to make it more concise. Below is a list of some of these features and, if possible, how they can be used to make the example more concise.

- **Prefix notation** allows us to shorten URIs by defining a prefix.
 - Using `@prefix schema: <https://schema.org/>` allows us to shorten `https://schema.org/Person` to `schema:Person`
- **Base prefix** allows us to shorten URIs by defining a base URI.
 - Using `@base <http://example.com/>` allows us to shorten `http://example.com/r0785695` to `r0785695`
- **Predicate lists** allow us to shorten multiple triples with the same subject to a list of predicates.
 - All our triples in the example are about `r0785695`, so we can split the predicates with `;` instead of repeating the subject.
- **Object lists** allow us to shorten multiple triples with the same subject and predicate to a list of objects.
 - `r0785695` is both a `Person` and a `Student`, so we can split the objects with `,` instead of repeating the subject and predicate.
- **Literals** allow identifying values, e.g. strings, integers, dates, etc. with a datatype or language tag.
- **Blank nodes** allow us to define anonymous resources by using the `_:` prefix.
 - The address of `r0785695` is only relevant to `r0785695`, so we can define it as a blank node instead of a URI, this shortens `<http://example.com/addr0785695>` to `_:addr0785695`.
- **Unlabeled blank nodes** allow us to define anonymous resources without a unique identifier by using the `[]` notation instead of `_:name`.
 - As we do not need to refer to the address of `r0785695` from outside `r0785695`, we can use an unlabeled blank node instead of a labeled blank node.
- **Collections** allow us to define a list of blank nodes by using the `()` notation.

The example in listing 2.1 can be rewritten using these features, as shown in listing 2.2.

```
<http://example.com/r0785695> <http://www.w3.org/1999/02/22-rdf-syntax-ns#
  type> <http://schema.org/Person> .
<http://example.com/r0785695> <http://www.w3.org/1999/02/22-rdf-syntax-ns#
  type> <http://schema.org/Student> .
<http://example.com/r0785695> <http://schema.org/givenName> "Tijs" .
<http://example.com/r0785695> <http://schema.org/familyName> "Van Kampen" .
<http://example.com/r0785695> <http://schema.org/address> <http://example.
  com/addr0785695> .
<http://example.com/addr0785695> <http://schema.org/postalCode> "2800"^^<
  http://www.w3.org/2001/XMLSchema#integer> .
<http://example.com/addr0785695> <http://www.w3.org/1999/02/22-rdf-syntax-
  ns#type> <http://schema.org/PostalAddress> .
<http://example.com/addr0785695> <http://schema.org/streetAddress> "
  Gentsesteenweg XXXX"@nl .
<http://example.com/addr0785695> <http://schema.org/addressCountry> "
```

Belgium" .

Listing 2.1: Basic naive turtle document

```
@prefix schema: <https://schema.org/> .
@prefix xsd: <http://www.w3.org/2001/XMLSchema#> .
@base <http://example.com/> .
<r0785695> a schema:Person, schema:Student ;
  schema:givenName "Tijs" ;
  schema:familyName "Van Kampen" ;
  schema:address [
    a schema:PostalAddress ;
    schema:postalCode "2800"^^xsd:integer ;
    schema:streetAddress "Gentsesteenweg XXXX"@nl ;
    schema:addressCountry "Belgium"
  ] .
```

Listing 2.2: Basic turtle document using turtle features

2.3 SPARQL

SPARQL Protocol And RDF Query Language (SPARQL) is the W3C standard query language for RDF. It is the main way to query RDF data and is similar to SQL. SPARQL queries mostly consist of a pattern of triples, which are matched against the RDF graph, a basic example can be found in listing 2.3. Querying is very feature-rich, with support for aggregation, subqueries, negation, etc. It also supports different return types, federated queries, entailment, etc. (Harris and Seaborne, 2013) Aside from the query protocol it also defines the graph store protocol, which can be used to manipulate graph databases directly (Aranda et al., 2013).

```
PREFIX schema: <https://schema.org/>
SELECT ?name ?address
WHERE {
  ?student schema:givenName ?name .
  ?student schema:address ?address .
}
```

Listing 2.3: Example of a basic SPARQL SELECT query

2.4 Mapping languages

Mapping languages are used to define a mapping between a source and a target. The target in the context of linked data is of course RDF, with the source being any structured data source. Some

mapping languages exist for a single source, e.g. Relational Database to RDF Mapping Language (R2RML) for relational databases, a query language combining XQuery and SPARQL (XSPARQL) for XML, etc. Others are more general purpose, e.g. RDF Mapping Language (RML) and Data to RDF Mapping Language (D2RML). We will discuss both R2RML and RML in more detail, as one extends the other. RML we will discuss because it is one of the more feature-rich general mapping languages, and it is the mapping language we will use in our implementation. R2RML we discuss because it is the most widely used mapping language, as it supports virtualization *ontop* of databases. Most RML implementations also support R2RML, as RML is a nearly superset of R2RML.

2.4.1 R2RML

Relational Database to RDF Mapping Language (R2RML) is a mapping language for mapping relational databases to RDF. As opposed to Direct Mapping (DM), which results in a direct mapping from the relational database to RDF without any changes to structure or naming, R2RML allows for more flexibility. R2RML mappings consist of zero or more TriplesMaps, which are used to map a table to RDF. A TriplesMap consists of a logical table, a subject map, and one or more predicate object maps (POMs).

The logical table is used to define the table that is being mapped, with each row in the table being mapped to a subject and its corresponding POMs. It is possible to create a view of a table by using a SQL query, and then map this view. This allows for more complex mappings, e.g. mapping a join of two tables or a computed column.

Each of the SubjectMap, PredicateMap, ObjectMap, (and GraphMap) is a subclass of TermMap, which is a function that generates an RDF term. The map type can be constant, template, or column. The resulting term is then used as the subject, predicate, object, or graph of the triple. The termType of the map determines the type of the term, which can be IRI, blank node, or literal. If the termType is literal, optionally the datatype or language can be added. Following the RDF specification, not all combinations of termType and map are possible, this is shown in table 2.1. The object map has an additional subclass, a reference object map, in which we refer to another TriplesMap. Using a reference map we can map a foreign key to the subject of another TriplesMap, with a join condition. (Cyganiak et al., 2012)

TermType	Subject	Predicate	Object	Graph
IRI	✓	✓	✓	✓
Blank node	✓	✗	✓	✓
Literal	✗	✗	✓	✗

Table 2.1 Possible combinations of TermType and Map type

A constant value is a fixed value, e.g. a URI or a string. A template is a string with placeholders, which are replaced by values from the logical row. A column is the value of a column in the logical row.

R2RML		RML	
Logical Table (relational database)	rr:logicalTable	Logical Source	rml:logicalSource
Table Name	rr:tablename	URI (pointing to the source)	rml:source
column	rr:column	reference	rml:reference
(SQL)	rr:SQLQuery	Reference Formulation	rml:referenceFormulation
per row iteration		defined iterator	rml:iterator

Table 2.2 Differences between R2RML and RML

@prefix rr: <http://www.w3.org/ns/r2rml#>.

@prefix ex: <http://example.com/ns#>.

```
<#TriplesMap1>
  rr:logicalTable [ rr:tableName "EMP" ];
  rr:subjectMap [
    rr:template "http://data.example.com/employee/{EMPNO}";
    rr:class ex:Employee;
  ];
  rr:predicateObjectMap [
    rr:predicate ex:id;
    rr:objectMap [ rr:column "EMPNO"; rr:datatype xsd:positiveInteger ].
  ].
```

Listing 2.4: Example of an R2RML mapping

2.4.2 RML

RDF Mapping Language (RML) is a mapping language for mapping any (semi-)structured data source to RDF. It is a generalization of R2RML and as such supports all the features of R2RML. It extends R2RML by extending database-specific features to make them more general. The differences in usage can be seen in table 2.2. (Meester et al., 2022)

RML uses the same structure as R2RML, with TriplesMaps consisting of a logical source, a subject map, and zero or more POMs. The changes it has all relate to the logical source. Whereas in R2RML the source is always a database, from which we select a table or view, in RML the source can be one of many different source types like XML, JSON, CSV, etc. Where in R2RML we simply iterate over the rows of a table, in RML we can have a source without an explicit iteration pattern, and as such we need to define an iterator.

Chapter 3

Implementation

This chapter is split into three sections. In the first section, we go over the structure of the algorithm. In the second and third sections, we go into detail about the two sub-research questions: how to construct the schema and how to populate the schema.

For the implementation, we assume that the mapping rules never map to a superset of the knowledge graph.

The implementation is written in Python. As we seek to extend Morph-KGC we make use of its internal functions and the libraries to work with those, like pandas. Querying the knowledge graph is done with the SPARQLWrapper library.

3.1 General structure

The algorithm consists of 4 main parts: setting up, creating the schema, retrieving the data, and applying the data to the schema. Creating the schema and retrieving the data are the two main parts of the implementation, and are covered in their sections. Setting up consists of setting up the SPARQL endpoint if necessary and processing the mapping files. Applying the data to the schema consists of applying the data of each iteration to the schema, and creating the output file. A graphical representation of the algorithm can be found in figure 3.1. A more formal representation can be found in algorithm 1.

3.1.1 Loading the mapping rules

We start by loading the mapping rules from the mapping files. We use Morph-KGC's internal `retrieve_mappings` function for this. This function takes a config file (.ini format) as input, which specifies the location of the mapping files and various other settings for which we have little use as they are only used for the materialization process. When relevant later on we could add our settings to this config file. The mappings are returned as a pandas DataFrame. As the pandas library has the functionality to group by columns, we can easily group the mapping rules by source and iterator later. An example of a single mapping rule (row in the DataFrame) can be found in listing 3.1.

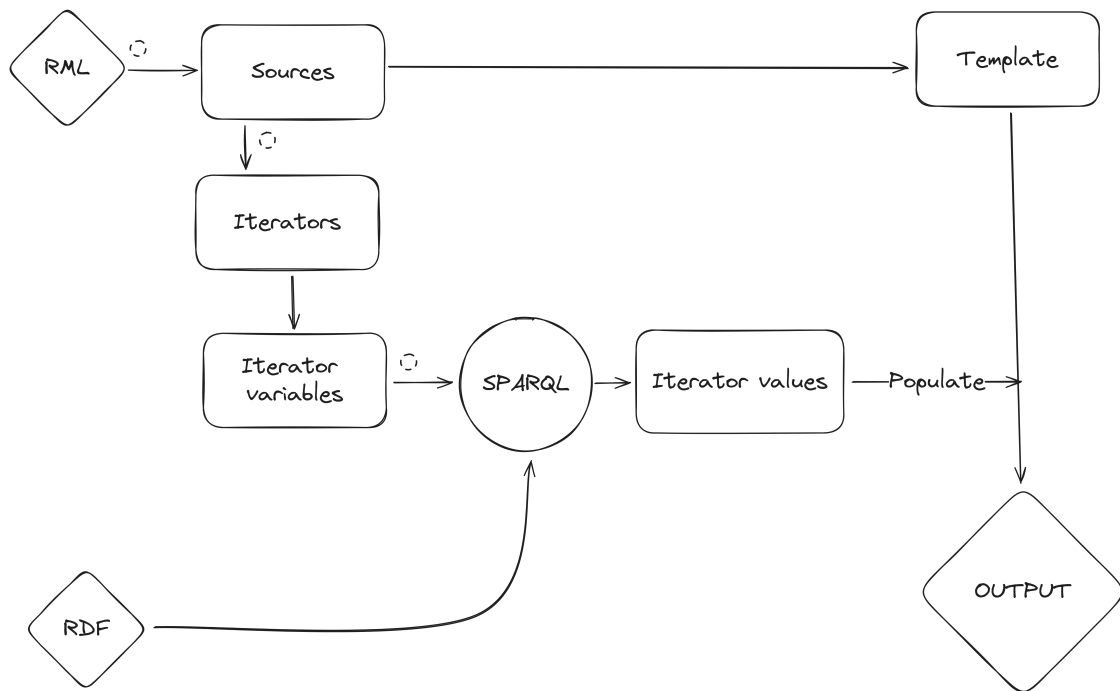


Figure 3.1: Overview of the algorithm

```

source_name: DataSource1
triples_map_id: #TM0
triples_map_type: http://w3id.org/rml/TriplesMap
logical_source_type: http://w3id.org/rml/source
logical_source_value: student.csv
iterator: nan
subject_map_type: http://w3id.org/rml/template
subject_map_value: http://example.com/{Name}
subject_termtype: http://w3id.org/rml/IRI
predicate_map_type: http://w3id.org/rml/constant
predicate_map_value: http://xmlns.com/foaf/0.1/name
object_map_type: http://w3id.org/rml/reference
object_map_value: Name
object_termtype: http://w3id.org/rml/Literal
object_datatype: nan
object_language: nan
graph_map_type: http://w3id.org/rml/constant
graph_map_value: http://w3id.org/rml/defaultGraph
subject_join_conditions: nan
object_join_conditions: nan
source_type: CSV
mapping_partition: 1-1-1-1

```

Listing 3.1: Example of a mapping rule in Morph-KGC

Algorithm 1 Inversion

```

1: optional(graph  $\leftarrow$  load_graph(rdf))
Require: mapping_files is a set of mapping files
Require: graph is a sparql endpoint
2: for all mapping_file  $\in$  mapping_files do
3:   mapping_rules  $\leftarrow$  parse_mapping_file(mapping_file)
4: end for
5: for all source, source_rules  $\in$  mapping_rules.groupby('source') do
6:   for all iterator, iterator_rules  $\in$  source_rules.groupby('iterator') do
7:     selected_rules  $\leftarrow$  get_optimal_rules(iterator_rules)
8:     for all subject, subject_rules  $\in$  selected_rules.groupby('subject') do
9:       query  $\leftarrow$  generate_query(subject_rules)
10:      values[iterator]  $\leftarrow$  graph.query(query)
11:    end for
12:  end for
13:  templates  $\leftarrow$  generate_templates(source_rules)
14:  source_output  $\leftarrow$  apply_templates(templates, values)
15: end for

```

3.2 Contructing the schema

Chapter 4

Evaluation

In this chapter we will evaluate our implementation. We will do this by testing it against various datasets, comparing the expected results with the actual results. For each dataset we will go over our testing methodology and its results.

4.1 RML test cases

The RML test cases are a set of test cases to evaluate the conformity of an RML processor. Though these test cases are not a perfect match, they offer expected outputs for certain inputs and mapping rules, making them a good starting point for testing our implementation. Tests that error do not produce a result, so we start by filtering those out.

Chapter 5

Conclusion

Placeholder chapter for referring to the conclusion chapter. This should be removed in the intermediate report.

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