

POLITECNICO DI TORINO

DEPARTMENT OF CONTROL AND COMPUTER ENGINEERING

Master of Science in Computer Engineering

Master Degree Thesis

Deep Learning on Academic Knowledge Graphs

Predicting new facts in a novel semantic graph built on top of the Politecnico di Torino scholarly data



Supervisors

Dr. Antonio Vetrò

Prof. Juan Carlos De Martin

Candidate

Giovanni GARIFO

ACADEMIC YEAR 2018-2019

To Monia
To my Grandfather

Abstract

The publication and sharing of new research results is one of the main goal of an academic institution. In recent years, many efforts have been made to collect and organize the scientific knowledge through new, comprehensive data repositories. To achieve such goal new tools that are able not only to store data, but also to describe them are needed.

Knowledge graphs are a particular class of graphs that are used to semantically describe the human knowledge in a specific domain by linking entities through labeled and directed edges.

In this work is presented a novel semantic graph built on top of the scholarly data produced by the Politecnico di Torino (Polito), and how state-of-the-art machine learning techniques have been used for the prediction of new links in this graph. Such graph, built by leveraging Semantic Web technologies, links together publications, researchers, fields of study and scientific journals in order to build a knowledge base that describes the Politecnico di Torino scientific community. This new academic graph has been called the *Polito Knowledge Graph*.

The prediction of non-existent links between graph nodes is one of the most challenging tasks in the field of statistical relational learning for graph data, mainly because, in order to obtain meaningful predictions, the vector representations of the entities must embed their semantic characteristics. To accomplish such goal, a deep neural network derived from the image recognition field and specifically adapted to the task of representation learning for graph data have been used. Such architecture allowed to obtain representations that have been directly learnt from the graph structure itself, without requiring any prior knowledge or feature engineering. Such representations allowed to obtain meaningful predictions that have been used to empower a recommendation system for the suggestion of useful insights.

Acknowledgements

I would like to express my deep gratitude to Giuseppe Futia, for his useful advices, his support in the revision of this work and his enthusiastic encouragement.

I would also like to express my gratitude to the supervisors of this work, Dr. Antonio Vetrò and Prof. Juan Carlos De Martin, for the useful comments and revisions.

Thanks also need to be made to all my colleagues of the Nexa Center for Internet & Society, who supported me during my master degree studies. Special thanks must be given to Marco Conoscenti and Selina Fenoglietto for the advices and support given during this years.

I also want to thank my family and friends, with a particular mention to Angelo Cataldo, friend of a lifetime.

This work is dedicated to Monia Fontana, without whose support I would not have been able to face the challenges that the life posed me in the latest years, and to my Grandfather, Giovanni Rotolo, passed away shortly after the start of my master degree, whom I hope to make proud by completing my university studies.

Contents

List of Tables	9
List of Figures	10
1 Introduction	11
1.1 Motivation	11
1.2 Goal and Contribution	12
2 Background	15
2.1 Semantic Web	15
2.1.1 From a Web of Contents to a Web of Data	15
2.1.2 The Semantic Web Building Blocks	16
2.1.3 Knowledge Bases as Knowledge Repositories	18
2.2 Learning on Graphs	21
2.2.1 Representation Learning	21
2.2.2 Deep Learning on Graphs	23
2.2.3 Link Prediction on Knowledge Graphs	26
3 Approach and Methodology	31
3.1 Builder Module	33
3.2 Enhancer Module	34
3.3 Viewer Module	35
4 Related Work	37
5 Development and Implementation	41
5.1 Building the Polito Knowledge Graph	42
5.1.1 PKG Ontology and Schema	43
5.1.2 The Graph Builder	45

5.2	Enhancing the Polito Knowledge Graph	49
5.2.1	The Dataset Builder	49
5.2.2	The Model Trainer	52
5.2.3	The Link Evaluator	58
6	Evaluation	61
7	Conclusions and Future Work	69
	Bibliography	73

List of Tables

2.1	Comparison of some of the biggest industry-scale knowledge graphs developed to this date. Table adapted from [1]. . .	19
5.1	Number of entities and edges in the Polito Knowledge Graph.	48
5.2	Statistics of the dataset produced by the Dataset Builder.	52
5.3	Hardware and software specifications of the workstation used to run the Model Trainer and the Link Evaluator. . .	54
6.1	Evaluation of different combinations of learning rate and regularization parameters using as benchmark the MRR value. The first table shows the MRR of the best model found during the training phase. The second table shows the MRR obtained by the best model over the test set. . .	63
6.2	Impact of the number of topics present in the RDF graph on the accuracy of the trained model.	66

List of Figures

2.1	An example of ontology defined using OWL and RDF Schema.	17
2.2	An extract of the Polito Knowledge Graph whose details will be described in section 5.1.	20
2.3	Word vectors allows to perform vector operations, the results obtained reflect the fact that Word2Vec is capable of embed the meaning of such words.	22
2.4	A digital image can be thought of as a graph.	23
2.5	Representation of a GCN updating the feature vector of the node 0 by summing the convolved features of its adjacent nodes.	26
2.6	R-GCN encoder visualization. Image taken from [2].	29
3.1	Schema of the pipelined software architecture developed to build, enhance and visualize the Polito Knowledge Graph. The legend is showed in the bottom left corner of the Figure. The circled numbers are used to identify the steps in the pipeline.	32
5.1	Schema of the Polito Knowledge Graph. The ontologies used to define the structure are shown in the prefixes table.	44
5.2	Visualization of the results obtained from the PKG when running a SPARQL query that returns all the publications that have <i>Knowledge Base</i> as topic. An excerpt of the RDF representation of this example will be listed in the following section.	45
5.3	Process of translation from RDF statement composed of URIs to edge tuple composed of integer indexes.	51
6.1	Number of triples for each ranking position obtained by evaluating the best model found over the test set. The ranking positions range from 1 to 47,995.	65

Chapter 1

Introduction

1.1 Motivation

Graphs are used to empower some of the most complex IT services available today, an example among all is the Google search engine¹. Graphs can be used to represent almost any kind of information, and they are particularly capable of representing the structure of complex systems and describe the relationships between their elements.

Over the last decade, much effort has been put in trying to leverage the power of graphs to represent human knowledge and to build search tools capable of querying and understanding the semantic relations within them. RDF² graphs are a particular class of graphs that can be used to build knowledge bases. Ontologies are used to shape such knowledge repositories, in order to have a semantically coherent representation of the domain knowledge. Given a domain and an ontology, RDF graphs allows to build a structured representation of the knowledge in such domain.

Modern machine learning techniques can be used to mine latent information from such graphs. One of the main challenges in this field is how to learn meaningful representations of entities and relations that embed the underlying knowledge. Such representations can then be used to evaluate new links within the graph or to classify unseen nodes. Deep learning

¹<https://blog.google/products/search/introducing-knowledge-graph-things-not/>

²The Resource Description Framework will be introduced in section 2.1.2

techniques have proved to be first class citizens when dealing with representation learning tasks, being able to learn latent representations without any prior knowledge other than the graph structure.

1.2 Goal and Contribution

Knowledge sharing is one of the main goals of research organizations. In particular, universities are among the most interested in making publicly available their research results. Today most universities have embraced the Open Science movement, making their scientific publications publicly available through web portals.

An example of such tools is the Institutional Research Information System (IRIS)³, an institutional publication repository developed by the Cineca Consortium and used by the Politecnico di Torino to store and share all the scientific papers published by its researchers.

IRIS allows to explore the published papers by searching for a field of study, matching it with the keywords inserted by the authors of the publications. The current implementation has some limitations: being inserted by the authors, the keywords can be acronyms, can contain abbreviations, initials written without capital letters, or misspelled words. In addition, they do not represent unique and field-wide semantic concepts, but they are simple character strings. The consequence is that the search engine of IRIS is unable to correctly retrieve all the publications about a specific research topic, because the system cannot match the searched field of study with an unambiguous *semantic entity*, but only with character strings that are not uniquely identified or semantically linked each other, and also prone to lexical errors.

The goal of this work is to overcome such limitations and enabling new possibilities for exploring and obtaining insights about the scientific community of the Politecnico di Torino. A new semantic-empowered search engine can be one of the possible solutions to obtain this results, allowing for coherent and precise results to be retrieved. At the foundations of this new semantic search engine there must be a data structure capable of representing semantic relations and concepts. Once such knowledge base of the scholarly data is obtained, it can be enhanced and completed by

³<https://iris.polito.it/>

automatically extracting latent information through the use of advanced machine learning algorithms.

In the next chapters is presented a newly built structured and semantically coherent representation of the scholarly data produced by the Politecnico di Torino, and how implicit facts can be automatically extracted from such knowledge repository by leveraging knowledge base completion techniques, implemented by means of an advanced link prediction algorithm.

Chapter 2

Background

2.1 Semantic Web

2.1.1 From a Web of Contents to a Web of Data

The World Wide Web has been developed as a tool to easily access documents and to navigate through them by following hyperlinks. This simple description already resembles the structure of a graph: documents can be thought of as nodes and hyperlinks as edges. The unstoppable growth of the *Web graph* led to the raise of new tools to explore such complexity. Search engines have been developed to easily navigate such a giant graph. First approaches were based on analytics evaluations, such as the number of times a document has been linked, as in the case of the PageRank [3] algorithm developed by Google.

The Web rapidly became one of the most innovative technology ever built, allowing to retrieve information quickly and easily as never before. The next evolutionary step has been to think about a Web not only exploitable by human beings but also by machines. In order to build such a comprehensive system, where information can be not only machine-readable, but machine-understandable, the World Wide Web had to move from a web of content, to a web of data.

The World Wide Web Consortium (W3C) introduced the Semantic Web as an extension to the prior standard of the WWW. Its primary goal has been to define a framework to describe and query semantic information

contained in the documents available on the Web, so as to allow machines to understand the semantic information contained in web pages. In the vision of Tim Berners-Lee, the father of WWW, this would bring to the transition from a World Wide Web to a Giant Global Graph¹, where a web page contains metadata that provides to a machine the needed information to understand the concepts and meanings expressed in it.

2.1.2 The Semantic Web Building Blocks

The three key components of the Semantic Web standard are:

1. OWL: the Web Ontology Language [4]
2. RDF: the Resource Description Framework [5]
3. SPARQL: The SPARQL Protocol and RDF Query Language [6]

OWL is a language used to define ontologies. In this context, an ontology is defined as a collection of concepts, relations and constraints between these concepts that describes an area of interest or a domain. OWL allows to classify things in terms of their meaning by describing their belonging to classes and subclasses defined by the ontology: if a thing is defined as member of a class, this means that it shares the same semantic meaning as all the other members of such class. The result of such classification is a taxonomy that defines a hierarchy of how things are semantically inter-related in the domain under analysis. The instances of OWL classes are called individuals, and can be related with other individuals or classes by means of properties. Each individual can be characterized with additional information using literals, that represent data values like strings, dates or integers.

The Resource Description Framework defines a standard model for the description, modelling and interchange of resources on the Web.

The first component of the framework is the *RDF Model and Syntax*, which defines a data model that describes how the RDF resources should be represented. The basic model consist of only three object types: resource, property, and statement. A resource is uniquely identified by an

¹<https://web.archive.org/web/20160713021037/http://dig.csail.mit.edu/breadcrumbs/node/215>

Uniform Resource Identifier (URI). A property can be both a resource attribute or a relation between resources. A statement describes a resource property, and is defined as a triple between a subject (the resource), a predicate (the property) and an object (a literal or another resource).

The second component of the framework is the *RDF Schema* (RDFS), that defines a basic vocabulary for describing RDF resources and the relationships between them. Many of the vocabularies and ontologies available today are built on top of RDFS, such as the Friend of a Friend (FOAF) ontology [7], for describing social networks, or the one maintained by the Dublin Core Metadata Initiative [8], that defines common terms and relations used in the definition of metadata for digital resources.

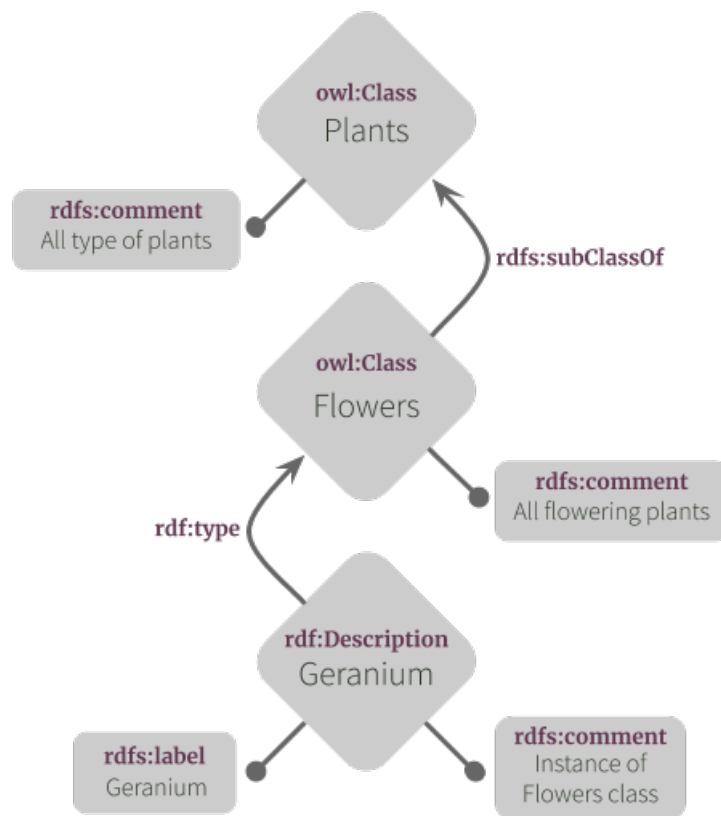


Figure 2.1: An example of ontology defined using OWL and RDF Schema.

SPARQL is a query language for triplestores, a class of Database Management Systems (DBMS) specialized in storing RDF databases. Such DBMS often expose endpoints that can be used to query the database

and obtain results. Given the complexity of the stored data, the query language has been designed to be as simple as possible, for instance by allowing the use of variables, whose definition is preceded by a question mark.

The syntax of SPARQL is heavily derived from SQL, with some minor adaptations to be more suited for querying graph data. The following is an example of query which selects all the labels (human-readable description of a resource) of all the entities that match the given resource type.

```
PREFIX plants:<http://example.org/plants/>

SELECT ?name
WHERE {
    ?subject rdf:type plants:flowers .
    ?subject rdfs:label ?name .
}
```

2.1.3 Knowledge Bases as Knowledge Repositories

Even though the raise of the Semantic Web has suffered a slowdown in its growth due to the complexity of its vision, many new projects were born from its enabling technologies. Efforts have been put by profit and non-profit organizations in trying to build complex knowledge repositories starting from the knowledge already available in the Web. An example among all is the DBpedia² project, which developed a structured knowledge base from the semi-structured data available on Wikipedia. Another example is the *Google Knowledge Graph*³, which is used to enhance the Google search engine and virtual assistant capabilities, allowing to retrieve punctual information about everything that has been classified in its ontology and described in its knowledge base, or the *Open Academic Graph*⁴, a Scientific Knowledge Graph that collects more than three hundred million academic papers. A comparison between some of the biggest

²<https://wiki.dbpedia.org/>

³<https://blog.google/products/search/introducing-knowledge-graph-things-not/>

⁴<https://www.openacademic.ai/oag/>

Table 2.1: Comparison of some of the biggest industry-scale knowledge graphs developed to this date. Table adapted from [1].

	Data model	Graph size	Development stage
Microsoft	Entities, relations and attributes defined in an ontology.	2 billion entities and 55 billion facts.	Actively used in products.
Google	Strongly typed entities, relations with domain and range inference.	1 billion entities, 70 billion assertions.	Actively used in products.
Facebook	All of the attributes and relations are structured and strongly typed.	50 million primary entities, 500 million assertions.	Actively used in products.
eBay	Entities and relation, well-structured and strongly typed.	100 million products, more than 1 billion triples.	Early stages of development.
IBM	Entities and relations with evidence information associated with them.	Various sizes. Proven on scales documents >100 million, relationships >5 billion, entities >100 million.	Actively used in products and by clients.

knowledge graphs developed to this date is available in Table 2.1.

From an implementation perspective, knowledge bases can be created by defining an ontology and a vocabulary for a specific domain of knowledge using OWL and RDF Schema, and then by describing the concepts of such domain using the RDF Model and Syntax. The RDF document obtained can then be stored in a triplestore and queried using SPARQL. The main effort in building knowledge bases is to have a correct understanding and prior knowledge of the domain of interest, to avoid the risk of mischaracterize or misrepresent concepts.

If all the requirements and precautions are met, a well formed knowledge base may prove to be a critical resource for an organization. It permits to build new services upon it, and also to improve the existing knowledge inside the organization by performing reasoning upon the available knowledge, in order to derive implicit facts starting from the existing entities and relationships. Another field of applications is the development

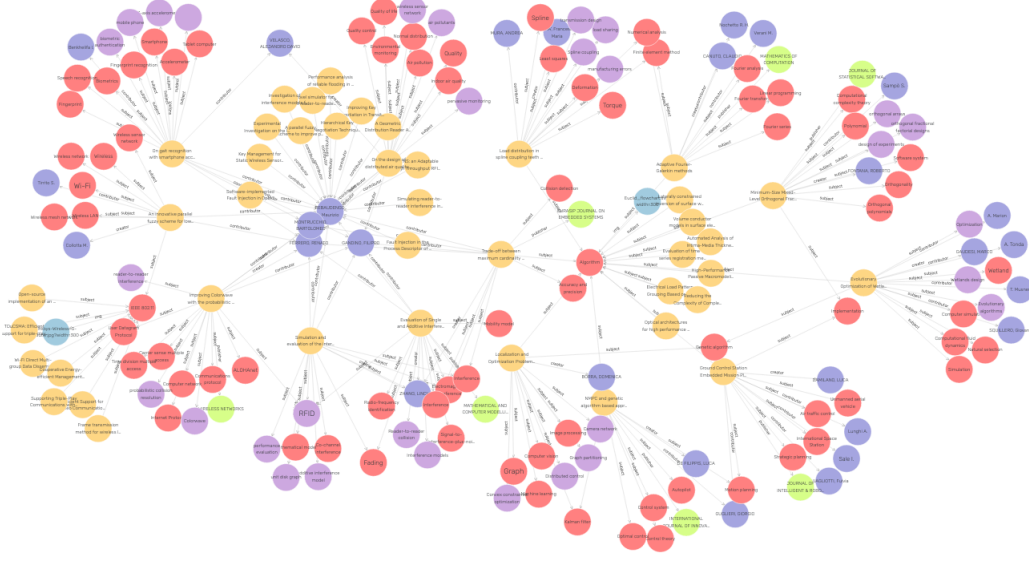


Figure 2.2: An extract of the Polito Knowledge Graph whose details will be described in section 5.1.

of Expert Systems⁵, AI software that emulates the behavior of a human decision-making process by navigating the knowledge base and taking decisions like in a rule-based system.

Today’s knowledge bases are commonly composed of tens of thousands nodes and by hundreds of thousands of edges. Considering such dimensions, storing and querying giant graphs requires the adoption of specialized DBMS that are capable of efficiently store and query the RDF input representation. Moreover, performing analysis and gathering statistics from such giant graphs requires the adoption of highly efficient algorithms in order to retrieve the desired output in an acceptable time.

The availability of such a complex and informative data structure leads to the opening of interesting scenarios, especially when thinking about the latent information that can be extracted from it. In fact, a knowledge base is a structured representation of the human knowledge in a specific field, thus its comprehensiveness is restricted by the human understanding.

⁵https://en.wikipedia.org/wiki/Expert_system

2.2 Learning on Graphs

2.2.1 Representation Learning

Machine learning (ML) algorithms are used to learn models from the available data, with the final goal to obtain a set of parameters that are fine-tuned to identify seen characteristics in the data used for training. The trained models can be used to recognize unseen inputs by leveraging the knowledge embedded in such parameters. An important task in the ML field is the learning of machine-understandable representations of the input data, task known as representation learning.

Natural Language Processing is one of the research branches that in the past years has made a great use of machine learning algorithms both for language recognition and for embedding words meaning into words vectors. One of the most successful algorithms when dealing with representation learning of words is Word2Vec [9], where the model obtained is trained to learn a vector representation for each word in a vocabulary. In Word2Vec, the concept of meaning of a word is related to the context in which such word is frequently used, so two words are recognized as similar if they are used in similar contexts. In the vector space of the learnt representations, words that have similar meaning have an higher cosine similarity⁶ with respect to the dissimilar ones. For instance, the cosine similarity between the word vectors of the words "Man" and "King" is roughly the same as the one between the words "Woman" and "Queen", since such words are used in similar contexts. This has open up new scenarios for language processing, since it allowed to perform vector operations on words vectors, which brought interesting results. An example can be seen in Figure 2.3.

This idea of words characterized by the context in which they're used can be generalized and applied to other fields of research, such as the field of representation learning on graphs.

Graphs are composed of nodes and edges, and are used to describe complex systems, such as social networks or the interactions in a molecular biology system. To apply machine learning algorithms to such data

⁶ Cosine similarity is a heuristic method to measure the similarity between two vectors by computing the cosine of the angle between them: $similarity(A, B) = \cos(\theta) = \frac{A \cdot B}{\|A\| \|B\|}$

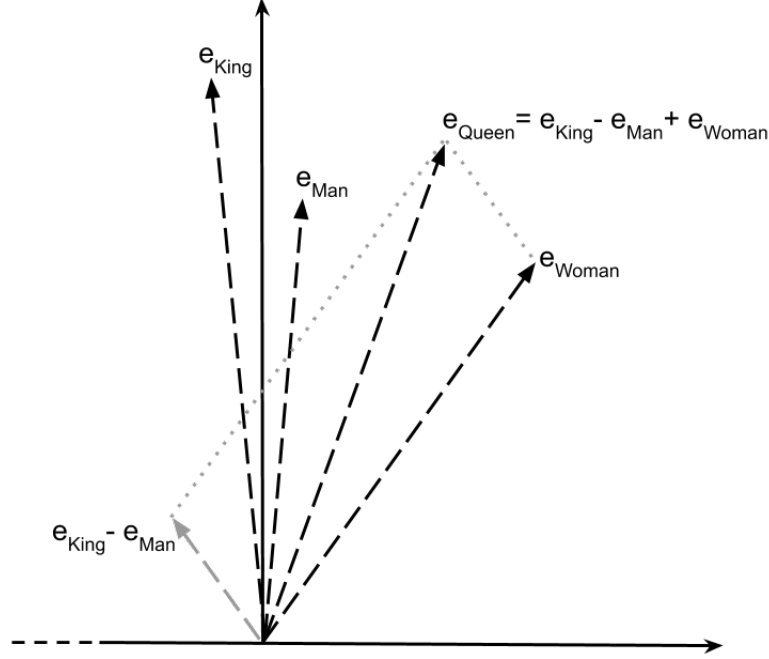


Figure 2.3: Word vectors allows to perform vector operations, the results obtained reflect the fact that Word2Vec is capable of embed the meaning of such words.

structures vector representations of nodes and edges are needed in order to be able to learn from the available data and predict new facts. Such vector representations are often referred to as *embeddings* because they should embed the characteristics of the graph nodes, so that similar nodes have similar embeddings. For instance, in a scholarly knowledge base publications with same authors and similar subjects should have similar embeddings.

Early approaches required these representations to be learned from feature vectors that were handcrafted, task that required not only a relevant amount of effort, but also a deep understanding of the domain of interest. This has long been one of the main obstacles when dealing with representation learning tasks, since who has knowledge of the domain and who has to engineer the features were unlikely the same individual.

2.2.2 Deep Learning on Graphs

In the latest years a big shift towards deep architectures has been made in machine learning, mainly thanks to the development of highly parallelized architectures that are able to efficiently compute at the hardware level vector and matrix multiplications, operations that are at the basis of any machine learning task. Deep learning algorithms are able to extract relevant features from raw data by applying simple mathematical operations, such as convolution, to the input data. An example of one of the most successful applications of deep neural networks is in image recognition, where matrix representations of images are convolved with self-trained filters that are able to extract the relevant features needed to recognize patterns present in the input images.

Deep learning techniques have proven to perform well also in the field of representation learning for graph data. As can be seen in figure 2.4, a digital image is composed of pixels which can be thought of as nodes in a graph, where each pixel is connected by an edge to its immediate neighbors. This suggests that the techniques used when dealing with images can be adapted, with some major changes, to the field of representation learning on graphs, but also in other fields of research, such as learning on manifolds.

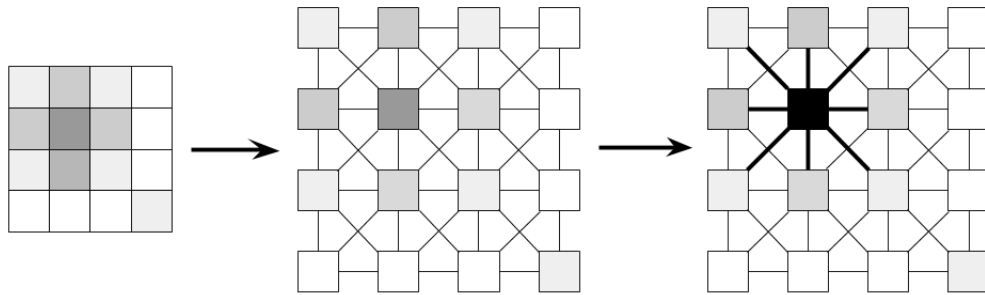


Figure 2.4: A digital image can be thought of as a graph.

One of the issues when working with graph data is that commonly graphs are built to describe complex systems, such as the knowledge of a domain or field for knowledge graphs, and thus are composed of a fairly high amount of nodes and edges. The matrices used to store the graph structure can thus explode in dimensionality, becoming impractical as input data. Moreover, graphs are not regular structures with a given

shape and size, such a matrix of pixels for images, but they live in an irregular domain which led to highly irregular structures. The first issue can be solved by randomly sampling the graph at each training epoch, the immediate drawback being that more than one epoch is required to train over all graph nodes. The second issue can instead be solved by adapting already existing algorithms to work on irregular domains. One of the possible approaches, which has proven to work well, is the one based on convolutions.

Graph Convolutional Networks (GCNs) [10] are a class of semi-supervised deep learning algorithms for graphs which are based on the same convolution and backpropagation operations as the well known Convolutional Neural Networks [11] (CNNs) used for feature learning on images. The main difference between CNNs and GCNs is in how the convolution is performed, instead the backpropagation phase is the same as the one used to update the parameters of CNNs, with a task-specific loss function. In a CNN the input matrix of each network layer, which is the pixel matrix of the input image for the first layer, is convolved with some layer-specific convolutional filters, whose parameters are then updated during the back-propagation phase.

GCNs works similarly by convolving at the l -th layer of the network the feature vector of each node with the feature vectors of its l -nearest neighbors by means of a convolutional filter. This operation is done by applying the following transformation:

$$H^{(l+1)} = \sigma(\tilde{D}^{-1/2} \tilde{A} \tilde{D}^{-1/2} H^{(l)} W^{(l)}) \quad (2.1)$$

Where $H^{(l)} \in \mathbb{R}^{N \times d^{(l)}}$ is the nodes hidden representation matrix, which is the output of the previous layer, with N being the number of nodes in the graph and $d^{(l)}$ being the dimensionality of the current layer. For the first layer, H^0 is equal to the input feature matrix X , where each row can be initialized with the respective node feature or with a one-hot encoded vector. For the last layer, $H^{(l+1)}$ is the embeddings matrix. \tilde{A} is an adjacency matrix of the graph that includes self loops. \tilde{D} is the node degree matrix of \tilde{A} and is used to normalize it. $W^l \in \mathbb{R}^{d^{(l)} \times d^{(l+1)}}$ is the convolutional filter that is shared among all nodes and is unique for each layer. The shape of this filter will directly impact the dimensionality of the embeddings obtained, in fact H^{l+1} is shaped as a $N \times d^{(l+1)}$ matrix. Finally, σ is a non linear activation function, for instance *ReLU*.

Looking at the update rule of a single node embedding will make more clear how the convolution is actually performed. The forward rule to update the embedding of a single node at the l -th layer of the network is the following:

$$h_i^{(l+1)} = \sigma\left(\sum_{j \in \eta_i} \frac{1}{c_{i,j}} h_j^{(l)} W^{(l)}\right) \quad (2.2)$$

Where η_i is the set of neighbors of node i , which contains the node itself because of the added self loop, and $c_{i,j}$ is a normalization constant obtained from the multiplication between the adjacency and degree matrices. The updated feature vector $h_i^{(l+1)}$ of the node i is obtained by performing the following operations:

1. The feature vectors $h_j^{(l)}$ of its neighbors are transformed by the matrix multiplication with the layer filter $W^{(l)}$.
2. The resulting $1 \times d^{(l+1)}$ shaped features vectors are multiplied with the respective normalization constants and summed together.
3. The non-linear function is applied to the result of the summation, obtaining the updated feature vector of the node i .

Applying such transformations to all nodes, at the k -th layer a node is represented by its transformed feature vector, which embeds the structural information within the node's k -hop neighborhood. As a consequence of this, the amount of layers of the network is an hyperparameter that controls how much information from furthest nodes has to be collected in each node embedding. This represents a fundamental architectural difference between CNNs and GCNs: while the former are commonly built by stacking a lot of layers, the latter relies on architectures that are more wider, due to the dimensionality of the graphs involved, and that consist of a fairly low amount of layers, in order to characterize the nodes only through their immediate surroundings.

As a result of the propagation step each node embedding will be characterized by its context, just like it happens in Word2Vec, but in a non-euclidean domain. So for example, in a social graph where each person is characterized by its friends, hobbies, places visited and so on, two people will have similar embeddings if they are both linked to the same nodes, and so they share the same interests and social connections.

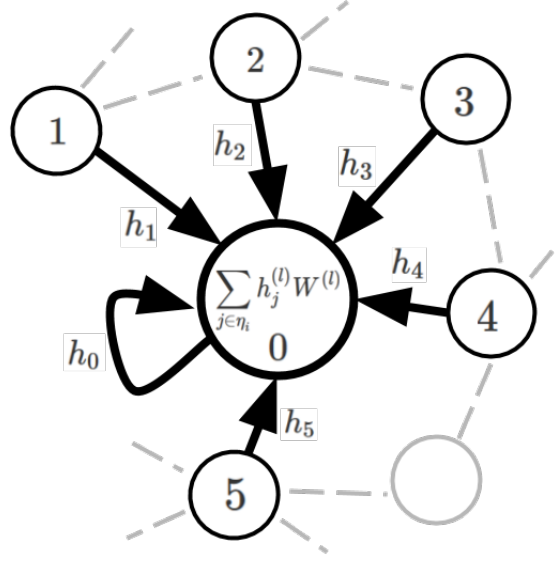


Figure 2.5: Representation of a GCN updating the feature vector of the node 0 by summing the convolved features of its adjacent nodes.

The node embeddings obtained by applying a GCN or one of its variants can then be used to perform some learning tasks on the graph, two examples are the classification of unseen nodes or the link prediction of non-existent edges. The latter is one of the most interesting tasks, since it allows to complete the information contained in the graph by predicting unseen facts.

2.2.3 Link Prediction on Knowledge Graphs

Predicting new facts is one of the most common task in the field of knowledge graph completion. The goal of such task is to predict new, unseen triples that correspond to missing facts in the knowledge base, and that can be later added to the graph. Deep learning techniques for link prediction are based on the following two main steps:

1. Train an *encoder* model that is able to embed the node features and produce meaningful embeddings.
2. Apply a factorization model that act as a *decoder*, which is used to score the unseen triples under evaluation.

Deep learning techniques such as GCN can be exploited to obtain meaningful node embeddings, but fall short when dealing with graphs where nodes are connected by different relations (multi-relational graphs). In fact, if a single layer GCN had been used to obtain the embeddings of two nodes that share the same neighborhood, but are connected to the neighbors via different relations, the resulting embeddings would have been very similar, even if it is clear that they do not share the same characteristics. For example in a producer-consumer framework one node could be the producer while the other the consumer, having both a common neighborhood of nodes which are produced by the former and consumed by the latter. If a GCN is used, the embeddings obtained would be very similar, even if the two nodes clearly do not have the same role and do not belong to the same class.

To overcome this limitation, changes to the basic GCN architecture have been proposed, so to obtain models that works well when applied to multi-relational graphs.

The Relational Graph Convolutional Network [2] (R-GCN) is an extension of GCNs which is focused on modeling multi-relational graphs composed by labeled and directed edges, and thus is particularly capable of embedding both nodes and relations of a knowledge graph. R-GCN can be used for both link prediction and node classification tasks.

At an high level the R-GCN architecture can be seen as a special case of the *message passing framework* [12], which groups together under a common scheme most of the existing neural models for graph data. The framework defines two major phases: a per-edge message computation and a per-node message reduction. In the first phase a function or linear transformation is applied to each edge to obtain an edge-specific message. Then, in the reduce phase, the embedding of each node is updated by aggregating together all the messages of the incoming edges.

This two phases can be grouped together through the following equation:

$$h_i^{(l+1)} = \sigma \left(\sum_{m \in \mathcal{M}_i} g_m(h_i^{(l)}, h_j^{(l)}) \right) \quad (2.3)$$

Where \mathcal{M}_i is the set of incoming messages for node i and g_m is a message specific transformation.

The idea behind the R-GCN is to have different set of parameters for different relations. At each step inside the network, the feature vector of a node is updated by convolving its first neighbors features with a convolutional filter that is different based on the kind of relation that connects the nodes. The forward rule to update the embedding of a node at the l -th layer is the following:

$$h_i^{(l+1)} = \sigma \left(W_0^{(l)} h_i^{(l)} + \sum_{r \in \mathcal{R}} \sum_{j \in \mathcal{N}_i^r} \frac{1}{c_{i,r}} W_r^{(l)} h_j^{(l)} \right) \quad (2.4)$$

Where $h_i^{(l)}$ is the embedding (or, for the first layer, the input feature vector) of the node i , $W_0^{(l)}$ is the learnt kernel for the self loop relation, \mathcal{N}_i^r is the set of indices of the neighbors of node i under the relation $r \in \mathcal{R}$, with \mathcal{R} being the set of all the relations present in the graph. $W_r^{(l)} \in \mathbb{R}^{d^{(l+1)} \times d^{(l)}}$ is the learnt filter for the relation r . As for the GCN architecture, σ is a non linear activation function and $c_{i,r}$ is a normalization constant, commonly initialized to $|\mathcal{N}_i^r|$.

From a message passing framework perspective, the message function (per-edge transformation) is equal to the linear transformation $W_r h_j$, and the reduce function (per-node transformation) is just the sum of all the messages computed for the edges connected to each node.

As can be seen the update rule looks similar to the one for GCNs (2.2), with the major difference that in the case of a R-GCN the filters used to convolve the feature vectors of neighboring nodes are relation-specific, so the number of filters at each layer will be equal to the number of relations inside the graph. As a consequence, the kind of relation that connect the node to its neighbors has an important role in determining the transformed node embedding.

Some form of regularization is required in order to avoid overfitting on rare relations, thus to obtain a more generalized model, and also to avoid the rapid growth in the number of parameters of the network for highly multi-relational graphs.

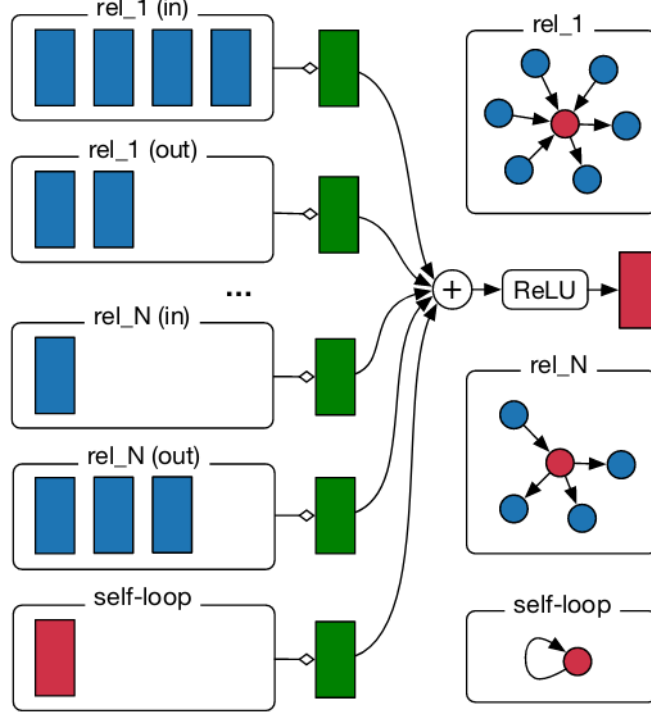


Figure 2.6: R-GCN encoder visualization. Image taken from [2].

One of the solutions proposed by the original paper [2] is to decompose each relation filter W_r using basis decomposition:

$$W_r^{(l)} = \sum_{b=1}^B a_{r,b}^{(l)} V_b^{(l)} \quad (2.5)$$

This allows to store only the relation-specific coefficients and the basis, which will be shared by all the relations.

The model obtained by training a R-GCN can then be used to build an encoder that given as input a graph, gives as output the embeddings of all nodes and the relations parameters. Then a factorization method can be used to evaluate unseen facts inside the graph, exploiting the resulting embeddings. Such methods are used as scoring functions in order to obtain, starting from the entities embeddings, a real value that can be used to score the unseen triples under evaluation.

DistMult [13] is one of the most common and simple factorization methods used to score unseen triples. Given a triple (s, r, o) , where s is the source node, o is the destination node, and r is the relation of the edge that links the source to the destination, DistMult allows to compute an associated real valued score as follows:

$$score_{(s,r,o)} = f(s, r, o) = e_s^T R_r e_o \quad (2.6)$$

Where e_s and e_o are the embeddings of the source and the destination node, obtained by means of an encoder model like R-GCN, and $R_r \in \mathbb{R}^{d \times d}$ is obtained by transforming the embedding of the relation r into a diagonal matrix. Such relation embedding is not learnt by the R-GCN encoder, but is a randomly initialized vector that represent the relation.

The score obtained by applying the factorization method above can then be used to evaluate whether the triple (s, r, o) is a good candidate to be added to the graph: an high score has to be interpreted as a high confidence of the model in the fact that the triple should belong to the knowledge base.

Chapter 3

Approach and Methodology

This chapter introduces the architecture developed to build, enhance and visualize the Polito Knowledge Graph (PKG), an academic RDF graph built to organize in a structured and semantically coherent way the publications produced by the researchers of the Politecnico di Torino. The graph also includes publication-related entities, such as authors, journals, and fields of study.

The architecture is composed of three main modules, that at an high level can be seen as part of a producers-consumers architecture, where the former produces the graph data, and the latter consumes it.

The architecture, which is shown in Figure 3.1, is structured as a pipeline composed of the following three modules:

1. The *Builder*, which creates a first version of the RDF graph.
2. The *Enhancer*, which implements ML techniques to predict unseen facts. Such facts can then be added to the graph in order to complete the knowledge base.
3. The *Viewer*, a web application that allows to query and visualize the graph data.

The *Builder* act as producer taking as input the IRIS data and producing a set of RDF statements that together composes the Polito Knowledge Graph. The *Enhancer* act as both a producer and a consumer, given that it takes as input the PKG and use it to predict unseen facts that can be

later added as new RDF statements. The *Viewer* consumes the graph by storing it a triplestore and exposing a public web interface for querying and visualizing the data.

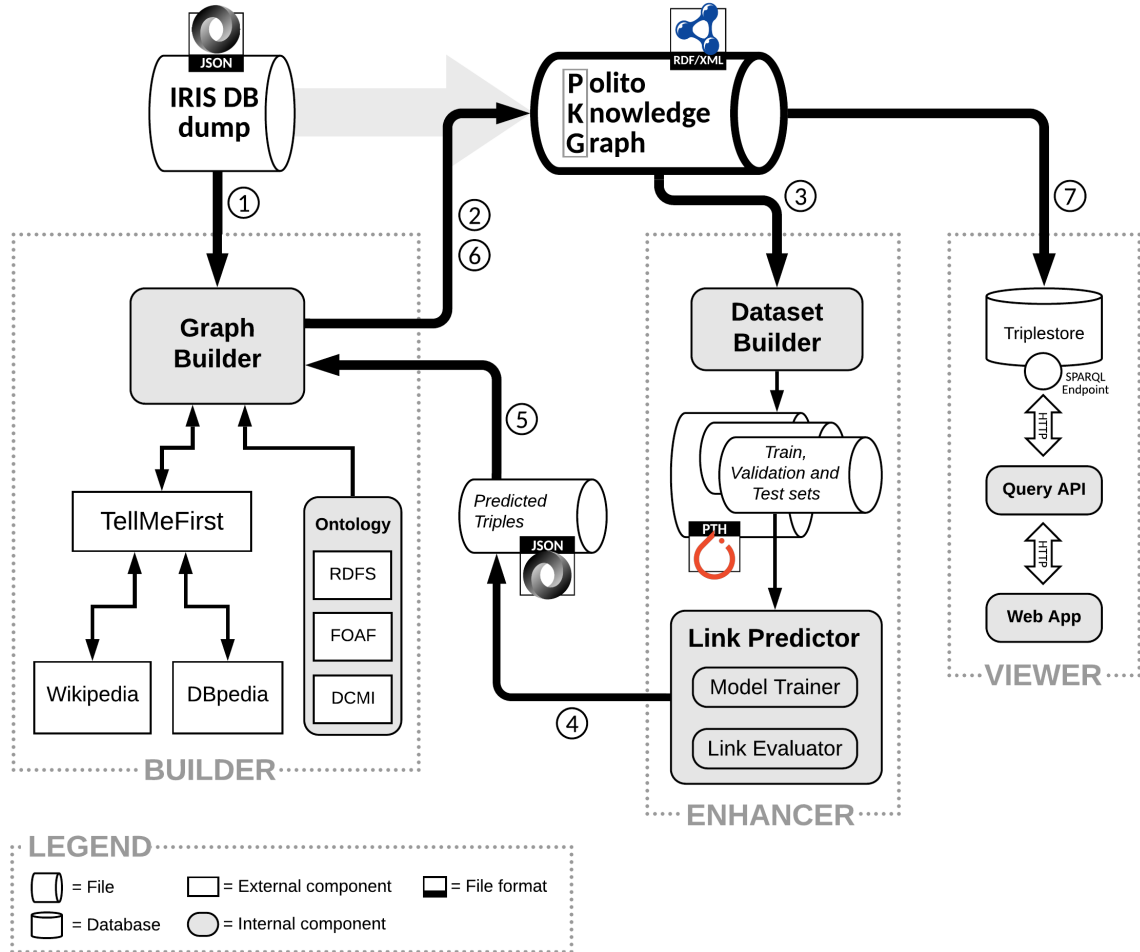


Figure 3.1: Schema of the pipelined software architecture developed to build, enhance and visualize the Polito Knowledge Graph. The legend is showed in the bottom left corner of the Figure. The circled numbers are used to identify the steps in the pipeline.

3.1 Builder Module

The Builder input is a dump of the IRIS¹ database, which is the platform used by the Politecnico di Torino to store and share all the scientific papers written by its researchers. The dump is a JSON file that contains all the information available for the scientific paper published in a period of five years that goes from 2013 to 2017.

The Builder goal is to translate all the information contained in the dump in a set of semantically coherent RDF triples. To do so, an ontology that describes the domain of the IRIS scholarly data has been defined.

The builder uses as reference the defined ontology to analyze each record in the JSON dump, and builds facts as RDF triples by matching the information contained in the record with the concepts defined by the ontology. For example, given that a publication may have more than one contributor, the defined ontology differentiates the principal author from the contributors by using two different statements to tie the corresponding entities to the publication.

One of the goal of this work is to link each publication to its research fields through unique and field-wide semantic concepts. To do so, the publication abstract has been used as input text for TellMeFirst (TMF) [14], a tool for the automatic extraction of semantic keywords from texts. Such semantic keywords, to which from now will be referred to as *topics*, are retrieved from the DBpedia taxonomy and are uniquely identified by their corresponding URI. The use of TMF allowed to automatically tie each publication to its relevant topics, by adding the corresponding RDF statements to the graph. Being the topics added as graph entities which are uniquely identified, all the publications that share a topic are linked to the same semantic entity.

The result of this process is a set of RDF statements that constitutes the first version of the Polito Knowledge graph, a semantically coherent description of the publications produced by the Polito researchers, where each publication is uniquely identified and linked by means of semantic relations to the entities representing its authors, contributors and research topics.

¹<https://iris.polito.it/>

3.2 Enhancer Module

Once the first version of the RDF graph has been built, it could be used as input for the Enhancer Module, whose main goal is to infer unseen facts to complete and enhance the information available inside the knowledge graph.

The Enhancer is composed of three main components:

1. The Dataset Builder.
2. The Model Trainer.
3. The Link Evaluator.

The Dataset Builder is in charge of translating the RDF graph into a usable dataset for the Model Trainer, this because the RDF statements cannot be used as input data for the link prediction algorithm. The dataset will then be splitted into three disjoint² sets.

The Model Trainer uses this three sets to train, validate and test the link prediction model. The training set is used to train the model at each epoch, while the validation set is used to evaluate which model parameters to keep, identifying the best epoch. The test set is used to evaluate the accuracy of the model, loaded with the best epoch parameters, upon unseen triples. Once the model has been trained, it can be used to predict unseen facts.

The Link Evaluator loads the best model found during the training phase and uses it to evaluate unseen triples. To do so, the Evaluator creates a set of unseen RDF triples and produces a score for each of them. Only the triples that obtain an high score (and so have an high probability to be true facts) and are correct in domain and range with respect to the ontology are kept. The predicted triples are then saved as RDF statements and could be added to the RDF graph, obtaining the enhanced version of the Polito Knowledge Graph. This new version will contain not only the information available on IRIS, but also the latent information inferred by the learnt model, like missing topics, similar authors or proposed journals, which can be used to empower a recommendation system for the Polito researchers.

²Two sets are said to be disjoint if they have no elements in common.

3.3 Viewer Module

The last module of the architecture is the Viewer, which is composed of a triplestore, an API layer, and a front end web interface.

The triplestore is a specialized DBMS for storing and retrieving RDF statements. It stores an online copy of the Polito Knowledge Graph and expose a SPARQL endpoint that allows to query the graph itself.

The API layer exposes a REST API that allows to retrieve the information contained in the graph without the need of using SPARQL queries. It accepts HTTP requests with URL-encoded parameters and proceeds to query the SPARQL endpoint of the triplestore by matching the parameters upon some predefined queries. Then, it translates the response obtained from the triplestore in a JSON file, which is sended back to the requesting client, which is typically the front end.

The front end is a responsive web application that act as the entry point for the user, mimicking the functionalities of a modern search engine. It allows to query and visualize the data contained in the graph through the use of a simple and friendly User Interface.

For example the user, who should typically be a researcher of the Politecnico di Torino, can search for a topic of interest and obtain as result the list of all the publications, authors and journals that are linked to such topic. The predictions are used to add suggestions to the results, for example, if searching for an author, in the results obtained are shown not only its actual research interestes, but also other topics in which he may interested in, or researchers with similar profiles but with which he never published a research together, thus obtaining useful insights about its scientific community.

Chapter 4

Related Work

Today there is a growing interest in scientific knowledge graphs, both from academic institutions and private organizations. An example is the Open Academic Graph¹ (OAG), an academic knowledge graph that has been built by merging together two of the largest scientific KG available, the Microsoft Academic Graph² and AMiner³. The OAG has been publicly released to allow the study of citation networks, papers content and more. The first version of the graph, released in 2017, has been built by merging together the aforementioned graphs and by linking the matching publications, obtaining a graph that is composed of more than three hundred million publications. In the first version of the graph the only kind of entity present was the publication: authors, journals, and all the other publications metadata were added as attributes, and not as entities.

In January 2019 the second version of the Open Academic Graph has been released, adding even more publications to the graph. However, the biggest change of this new version was the addition of authors and venues as graph entities, instead of being simple publications attributes.

However, the OAG does not contain the publications topics as graph entities, but as author keywords, thus being prone to the same limitations of IRIS: the keywords are the ones chosen by the authors and are not referencing to semantic concepts, being simple character strings.

¹<https://www.openacademic.ai/oag/>

²<https://academic.microsoft.com/>

³<https://www.aminer.cn/>

Regarding the development of tools similar to the Polito Knowledge Graph by other academic institutions, an example of employment of knowledge graphs and natural language processing techniques to build new academic search engines is Wiser [15], an expertise search tool developed by the University of Pisa and publicly released at the beginning of 2019. The knowledge graph of Wiser is composed of approximately 1,500 authors, 65,000 publications and 35,000 topics⁴. The system has proven to be particularly effective, representing a strategic tool and being actively used by the university Technological Transfer Office to easily find expertise profiles in a given research field.

As saw in the previous Chapter, one of the main components of the PKG pipeline is TellMeFirst, tool used to automatically extract the topics of interest from the publications abstracts. By automatically extracting the topics, TMF allows to add them as entities in the Polito Knowledge Graph, so that each publication is directly linked to its main topics, and each topic is linked to all the publications of which it is a subject (reverse relation).

Other tools that are able to extract the subjects of a publication exists, an example is the CSO Classifier [16]. This tool is able to automatically classify a research paper according to the Computer Science Ontology⁵ (CSO), an automatically generated ontology of research topics in computer science. The fact that the CSO Classifier relies on a predefined ontology has some disadvantages with respect to TellMeFirst, the biggest being the fact that the Computer Science Ontology is restricted to the computer science field only, while TMF, using DBpedia as its source of knowledge, is able to extract topics (and so to classify a research paper) regarding every field of research. However, the approach of CSO Classifier has also its advantages: being the ontology more restricted, the classification could be more accurate, and the structure of the ontology itself may be tailored for such classification task.

Regarding the learning task on graph data, many architectures that implements the Message Passing Framework [12] and that are derived from

⁴Details about the Polito Knowledge Graph dimensionality and scale will be presented in the following chapter.

⁵<https://cso.kmi.open.ac.uk/home>

the classical Convolutional Neural Network are available, some example being [17] and [18]. However, the R-GCN architecture is employed for the learning task of this work, being specifically designed to work with relational graph data. Moreover, due to the different approach followed by the authors of R-GCN, which relies on the convolutional architecture only as an encoder, different factorization methods could be tried in future work while keeping the same encoder architecture based on the R-GCN. Some possible factorization methods that could be implemented as decoders are [19] and [20].

Chapter 5

Development and Implementation

In the first part of this chapter is described the development and the implementation of the Polito Knowledge Graph, particularly focusing on the components in charge of the graph creation and enhancement, whose architecture has been introduced in [Chapter 3](#).

Firstly, a detailed description of the input data used to create the graph is introduced, together with a description of the ontology used to shape the knowledge of the scholarly domain, and the graph schema obtained by structuring the information made available by IRIS with such ontology. Then, the implementation of the Builder Module is discussed. This module is responsible for the actual creation of the Polito Knowledge Graph starting from the IRIS publications metadata.

In the second part of the chapter the implementation of the link predictor module, which is used to predict new facts inside the knowledge base, is presented. Then is described how, starting from the Polito Knowledge Graph, a usable dataset for the training of an encoder model has been obtained, which architecture and hyperparameters are used, how the model has been trained and how it has been validated during the training phase in order to choose the best parameters. It will also be discussed how the model has been tested, and which metrics have been used to evaluate the accuracy of the predictions on the test set.

Finally, is presented how the trained model have been employed for the prediction of new facts, and how the predictions obtained can be used to build a recommendation system for the Polito Knowledge Graph.

5.1 Building the Polito Knowledge Graph

As already mentioned when introducing the pipeline in Chapter 3, the input data used to build the PKG is a dump of the IRIS database, which contains the information about the scientific papers published by the researchers of the Politecnico di Torino in a five-year period. The dump is a JSON file composed of 23,268 records, and each record contains the metadata of a single scientific publication. Many of the available metadata are generated by the IRIS platform, in order to manage its internal processes of publications management. Such information have been discarded, since they are not significant for the publication characterization.

The following metadata have been selected as the ones that truly characterize a scientific paper:

1. The publication identifier.
2. The title.
3. The abstract.
4. The author name, surname and identifier.
5. The contributors and coauthors names, surnames, and identifiers (if present).
6. The date of publication.
7. The journal title and ISSN (if present).
8. The keywords entered by the authors to tag the publication.

The publication identifier is a unique numeric code associated by IRIS to each scientific paper. Also the authors, contributors and coauthors should be uniquely identified by an alphanumeric identifier, however, only the researchers of the Politecnico di Torino have such identifier. External researchers that may be contributors or coauthors of the publication are present with only their name and surname. The author is instead always a Polito researcher.

If the scientific paper has been published in a journal, the journal ISSN is used as identifier, if present. If the paper is available in a conference proceeding, no information about the conference is present other than the title, thus it is not possible to uniquely identify it, at least not in this first version of the Graph Builder. The publication title, the abstract, the

names, surnames and the keywords and the date of publication are simple character strings.

As already discussed in previous Chapters, the keywords entered by the authors cannot be treated as semantic concepts. To solve this issue TellMeFirst (TMF), a tool previously developed at the Nexa Center for Internet & Society, has been used. TMF allows the automatic extraction of semantic keywords from an input text, relying on the DBpedia ontology and knowledge graph as its source of knowledge. Using TMF it has been possible to extract the relevant topics from the publications abstracts, allowing to link the papers to the same unique and unambiguous semantic entities.

In the following sections is described how the Graph Builder has been developed, and how, leveraging TellMeFirst, the relevant topics of a publication have been extracted from the publications abstracts, in order to add such topics as uniquely identified graph entities in the Polito Knowledge Graph.

5.1.1 PKG Ontology and Schema

Starting from the metadata discussed above, the PKG ontology has been defined as composed of the following five different classes:

1. The *Publication*.
2. The *Author*.
3. The *Journal*.
4. The *AuthorKeyword*.
5. The *TMFResource*.

In order to build a knowledge graph, the instances of such classes must be linked together by means of semantic relations, called predicates. To do so, some predicates already defined by the FOAF [7] and the DCMI [8] ontologies have been used, together with some terms defined by the RDFS [5] standard. The graph structure obtained is represented by the schema in Figure 5.1, where are shown the classes, the attributes of such classes and the predicates that links them together.

As can be saw from the schema shown in Figure 5.1, the *Publication* class is linked to the *Author* class by means of two relations both defined

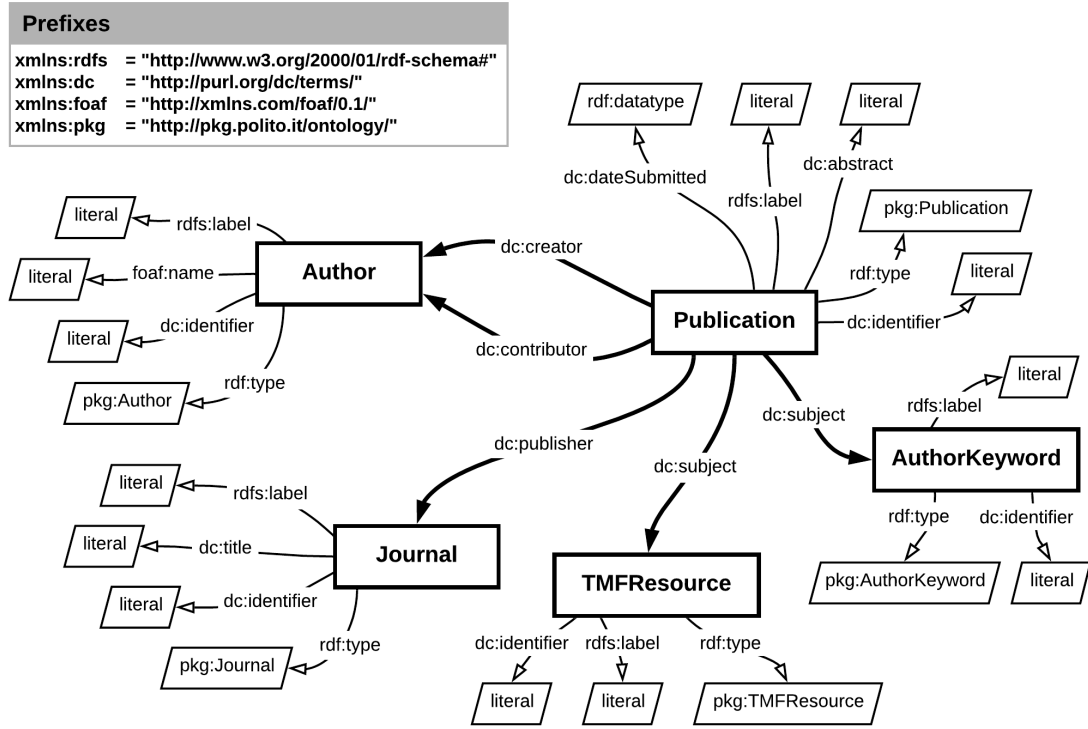


Figure 5.1: Schema of the Polito Knowledge Graph. The ontologies used to define the structure are shown in the prefixes table.

by the DCMI ontology: *dc:creator*¹ and *dc:contributor*¹.

Only the first author (*creator*) is differentiated from the others (*contributors*) due to the inability to discriminate, based on the metadata made available by IRIS, which are the co-authors and which are the collaborators.

The *AuthorKeyword* class represents the keywords added by the authors to tag the publication. Even if such keywords do not represent any semantic information, they are still added to the knowledge base for the sake of completeness with respect to the metadata available.

Instead, the *TMFResource* class is used to categorize the entities corresponding to the DBpedia resources extracted by TMF starting from the publications abstracts. Being uniquely identified by their DBpedia URI, the publications that shares a topic will be linked, through the *dc:subject*

¹The *dc* keyword is used as prefix for the Dublin Core Metadata Initiative (DCMI) namespace: <http://purl.org/dc/terms/>

relation, to the same instance of the *TMFResource* class that represents such topic. An example is shown in Figure 5.2, where are depicted all the publications that are linked to the entity instantiated for the *Knowledge Base* topic.



Figure 5.2: Visualization of the results obtained from the PKG when running a SPARQL query that returns all the publications that have *Knowledge Base* as topic. An excerpt of the RDF representation of this example will be listed in the following section.

5.1.2 The Graph Builder

The Graph Builder is implemented as a Python command-line script that uses the *rdflib*² library to create and manage an in-memory RDF representation of the graph. Such representation can be then serialized and saved as an XML file. The script takes as arguments the path to the JSON dump of IRIS, together with some options that allows to trigger specific functionalities of the script, such as:

²<https://github.com/RDFLib/rdflib>

1. The update of an already existing RDF graph with new statements, used for example to add the predicted triples.
2. The number of topics that must be extracted from each abstract by TMF, the default value is seven.
3. The addition of the URLs of the topics pictures, which are scraped from Wikimedia Commons³ through its publicly available SPARQL endpoint and added to the corresponding *TMFResource* instances.

The Graph Builder firstly declares the namespaces and the ontology used to define the RDF representation of the entities and the relation inside the graph as written in the previous section, then parses the arguments and options received and execute the corresponding activities.

If the creation of a new graph is requested, the script reads the JSON dump in a Python list and instantiates a *ThreadPoolExecutor*, a Python abstraction that allows to execute a function asynchronously by spawning a predefined number of threads. Each thread asynchronously executes a function that process a single record of the dump. The concurrent access to the records list is not a problem, being the Python lists implemented as thread safe containers. Each record is processed by:

1. Matching the record metadata with the ontology classes and creating the corresponding entities.
2. Requesting to TMF, via its API, the extraction of the topics from the publication abstract.

In the first step, when a field that matches a class is found, a corresponding RDF triple that creates a new entity is added to the graph. If the entity is already present, an RDF triple that connects the publication to the already existing entity is added.

The topic extraction is performed by TMF by sending an HTTP POST request containing the publication abstract and the requested number of topics to be extracted. The response contains the list of the DBpedia resources that TMF extracted as main topics for the publication. Such topics are added to the graph as *TMFResource* entities, and are linked to the publication by means of the *dc:subject* relation.

³<https://commons.wikimedia.org/>

Even if the Python interpreter implementation poses some limitations in the actual advantage of executing multithreaded code in CPU bound scenarios, in this case the use of multiple threads improved the time required to build the graph, being the implementation I/O bound by the communication with the REST API of TMF.

The two steps described above allows to generate the RDF description of a publication starting from its metadata, which is then enriched by the topics extracted by TMF.

Listing 5.1: Example RDF output of the Graph Builder.

```

1 <?xml version="1.0" encoding="UTF-8"?>
2 <rdf:RDF
3   xmlns:dc="http://purl.org/dc/terms/"
4   xmlns:foaf="http://xmlns.com/foaf/0.1/"
5   xmlns:rdf="http://www.w3.org/1999/02/22-rdf-syntax-ns#"
6   xmlns:rdfs="http://www.w3.org/2000/01/rdf-schema#"
7   xmlns:pkg="http://pkg.polito.it/"
8   xmlns:dbpr="http://dbpedia.org/resource/"
9   xmlns:xm1s="http://www.w3.org/2001/XMLSchema#">
10
11   <rdf:Description rdf:about="pkg:publications/2679709">
12     <rdf:type rdf:resource="pkg:ontology/Publication"/>
13     <dc:identifier>2679709</ns1:identifier>
14     <rdfs:label>Title</rdfs:label>
15     <dc:abstract>Abstract of the publication</ns1:abstract>
16     <dc:subject rdf:resource="dbpr:Knowledge_Base"/>
17     <dc:creator rdf:resource="pkg:authors/rp00000"/>
18     <dc:dateSubmitted rdf:datatype="xm1s:date">
19       2017-01-01
20     </dc:dateSubmitted>
21   </rdf:Description>
22   <rdf:Description rdf:about="dbpr:Knowledge_Base">
23     <rdf:type rdf:resource="pkg:ontology/TMFResource"/>
24     <rdfs:label>Knowledge Base</rdfs:label>
25   </rdf:Description>
26   <rdf:Description rdf:about="pkg:authors/rp00000">
27     <rdf:type rdf:resource="pkg:ontology/Author"/>
28     <foaf:name>Surname, Name</foaf:name>
29     <dc:identifier>rp00000</dc:identifier>
30     <rdfs:label>Surname, Name</rdfs:label>
31   </rdf:Description>
32 </rdf:RDF>

```

Table 5.1: Number of entities and edges in the Polito Knowledge Graph.

Polito Knowledge Graph				
Number of entities per-class				
Publication	Author	Journal	TMFResource	AuthorKeyword
23,268	34,886	3,211	16,988	41,807
Number of edges per-relation				
Creator	Contributor	Publisher	Subject (TMF)	Subject (Keywords)
23,268	80,819	11,243	107,093	77,492

For instance, the Listing 5.1 contains an example RDF description generated by the Graph Builder. As can be saw, not only a new publication entity is created, but also the author and the extracted topic are added to the graph and linked to the publication.

By translating every record of the IRIS database dump into a set of RDF statements, an RDF graph composed of entities that are uniquely identified and linked together by meaningful relations is created. The resulting graph is thus a comprehensive representation of the Politecnico di Torino academic community. The Polito Knowledge Graph links together researchers, their fields of interest, the scientific papers produced by them and the journals in which such papers have been published.

In Table 5.1 are summarized some statistics about the size of the PKG, showing the number of entities categorized under each class, and the number of edges for each relation type.

After all the publications have been processed by the Graph Builder, the internal representation of *rdflib* can be serialized and exported as an XML file that contains the definition of all the RDF triples that forms the Polito Knowledge Graph. Such RDF representation can be then used as input for the Enhancer Module or loaded into a triplestore (for example Blazegraph⁴) in order to be queried by the viewer component.

⁴<https://blazegraph.com/>

5.2 Enhancing the Polito Knowledge Graph

Once the first version of the Polito Knowledge Graph has been built, the Enhancer Module can be used to infer new facts. In this Chapter is presented how, starting from the RDF graph, a usable dataset for the learning task is created, how the employment of a R-GCN architecture allowed to encode the entity characteristics into meaningful embeddings and how the predicted triples have been obtained and evaluated.

5.2.1 The Dataset Builder

The Model Trainer can not learn the nodes embeddings by directly taking as input the RDF representation of the graph. To solve this issue, another component, the Dataset Builder, is in charge of creating a useful dataset for the learning task.

As discussed in the previous Chapter, some of the metadata available in the IRIS publications records are not uniquely identified, however, they have been still added them to the graph for the sake of completeness. As a consequence of this, the corresponding entities do not represent unambiguous semantic information, the effect being that such entities may only add noise to the dataset, thus leading to incorrect predictions.

To avoid this issue, only the entities which are unique and unambiguous in the whole graph are included into the dataset:

1. The publications, identified by their IRIS ID.
2. The authors, identified by their Politecnico di Torino internal ID.
3. The journals, identified by their ISSN.
4. The topics extracted by TMF, identified by their DBpedia URI.

With respect to the full set of entities of the Polito Knowledge Graph, all the external contributors and co-authors have been discarded, for which the only information available are their names and surnames, and also all the authors keywords. The dataset is thus built from a reduced version of the initial graph.

In the following, is explained how a usable dataset for the learning task have been built starting from such reduced version of the graph.

Like the Graph Builder, also the Dataset Builder is implemented as a Python command-line script that process the RDF graph triples with *rdflib*, which offers a practical interface to work with RDF data. The Dataset Builder has to convert the RDF representation of the graph into an integer representation, where each class, entity and relation has a corresponding integer index assigned.

The following input data are needed by the Model Trainer to train the encoder:

1. The number of nodes, equal to the number of RDF entities in the graph.
2. The number of different relations that links together the graph entities.
3. The number of nodes labels, where each label is referred to a class of the PKG ontology.
4. A list of edges, where each edge is a Python tuple composed of three elements: the node index of the subject and the object, and the index of the predicate. How such indexes are generated is explained in the following.
5. A list of node-specific normalization constants.

To build such data structures starting from the RDF graph, the Dataset Builder leverages some look-up hash tables (implemented as Python dictionaries) that are created starting from the RDF statements and the PKG ontology. Such tables are accessed by URI, and allow to retrieve the corresponding entity or relation integer index.

1. The *nodes table* is populated by assigning to each entity a unique, increasing integer index. Such index will identify the entity when building the list of edges. Only the entities that are instances of the classes that have been selected as part of the dataset are added to the table.
2. The *relations table* is built starting from the PKG ontology, assigning to each relation inside the graph a corresponding integer identifier.

When building such tables, the Dataset Builder also keeps track of the total number of nodes and relations, and builds a labels list that stores in the i -th element the class (label) of the i -th node.

Once the look-up tables and the other data structures are built, the Dataset Builder starts to process the RDF statements that composes the graph by looping through them.

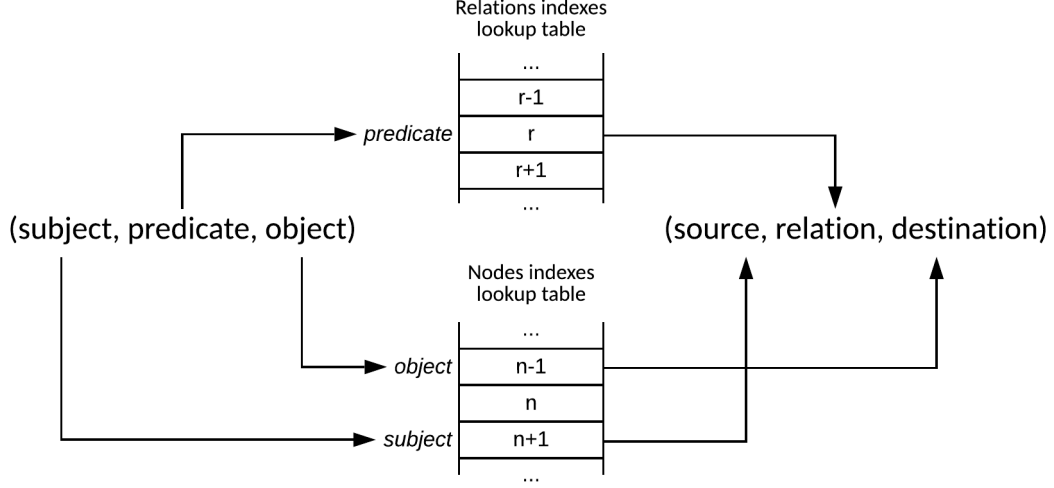


Figure 5.3: Process of translation from RDF statement composed of URIs to edge tuple composed of integer indexes.

For each statement, The Dataset Builder firstly checks whether the subject and object of the statement are present in the nodes table, if so, it builds the corresponding edge tuple by retrieving the indexes of the entities and relation through the look-up table. An example of this process is shown in Figure 5.3.

The obtained list of edges is then splitted into three separate and disjoint sets that will be used to train, evaluate and test the encoder model, making sure to have in the training set, for each node, at least one edge for every kind of relation present in its directly connected edges. This is mandatory to obtain meaningful embeddings, because as already explained in section 2.2.3, the R-GCN model learns the vector representations of the nodes by embeddings the nodes neighbors features. As a consequence of it, is crucial to have a neighborhood structure in the training graph which is similar to the one in the full graph. Once such initial sampling has been done, the remaining training edges are randomly taken.

The percentage of tuples used to create the three sets is an hyperparameter that can be chosen in advance. However, some tests showed that picking less than 70% of nodes for training does not allowed to maintain a representative neighborhood for each node, resulting in an inaccurate

Table 5.2: Statistics of the dataset produced by the Dataset Builder.

Dataset			
Number of nodes	Number of classes/labels	Number of relations	Total number of edges
47,996	4	4	170,593
Number of train, evaluation and test samples			
Train edges	Evaluation edges	Test edges	
153,531	8,528	8,534	

link prediction model. To solve this issue, the edges list is splitted in approximately 90% of the tuples for train, 5% for the validation and 5% for testing.

Once the dataset have been created and the list of edges splitted into the three sets, it is serialized and saved, so that for future run of the Model Trainer is not required to create the dataset from scratch. Moreover, since a part of the edges are randomly picked, this allowed to evaluate the different hyperparameters values upon the same set of triples.

Table 5.2 summarizes the characteristics of the dataset obtained by the Dataset Builder. The size of the dataset, in particular the number of nodes and edges, can be compared to the size of the initial RDF graph, whose statistics are available in Table 5.1. As can be saw, more then half the nodes, the ones referred to the author keywords and the external authors, have been removed.

5.2.2 The Model Trainer

Modern machine learning algorithms are implemented as deep networks composed by many layers and parameters. Building such architectures from the ground-up would be almost unfeasible, especially when dealing with challenging kinds of data structures, such as multi-relational graphs. Many frameworks and libraries that allow the implementation of complex architectures without the need of coding them from scratch. Moreover, one of the key aspects when coding machine learning models is to build highly efficient implementations, especially when working with giant data structures, as in the case of knowledge graphs, thus leveraging highly

optimized and tested software is crucial.

One of the most common used frameworks that allows to build and train ML models is PyTorch [21]. The goal of PyTorch is to provide some simple yet expressively powerful components that could be used to implement any sort of neural network, simplifying some of the most challenging aspects, like the implementation of the backpropagation phase. The two major abstractions introduced in the framework are the *tensor* and the *autograd*. Tensors are the basic data structure in PyTorch, they support both CPU and GPU execution and all the major operations for multidimensional matrices. The autograd package is the key novelty of PyTorch, allowing to perform automatic differentiation of all the operations performed on tensors by leveraging an internal representation in the form of a computational graph. However, even if PyTorch provides all the building blocks for developing complex neural networks, it is not suitable when dealing with graph data due to the lack of support for the message passing paradigm (which has been introduced in Chapter 2.2) by the tensor interface.

Deep Graph Library [22] (DGL) provides a more comprehensive solution specifically designed to work with graph data. DGL is built on top of existing ML frameworks (e.g. PyTorch, MXNet), and offers a simple interface that facilitate the implementation of the message passing framework. Supporting such framework, with DGL is possible to implement every deep learning algorithm whose forward pass can be divided into a per-edge message computation and a per-node message aggregation. Some of the architectures that can be implemented are depicted in [12], with R-GCN being one of them.

With DGL, a graph can be created by instantiating an object of the *DGLGraph* class, which offers a dictionary-like interface for adding to the graph both nodes and edges, together with their features or any other relevant data for the training, for instance the normalization constants. The message passing paradigm is implemented by means of the *send* and *recv* functions, which allows to define the two basic operations for the per-edge messages construction and the per-node aggregation.

As already mentioned before, the R-GCN architecture has been chosen to build an encoder model which is capable to produce the nodes embeddings starting from the graph structure. Later in this Chapter is discussed how the encoder model has been trained, how it has been implemented

with DGL, which learning problem the model had to solve and how it has been evaluated, so to chose the best parameters for the learning task.

To train and test the model a workstation whose hardware and software specifications are summarized in Table 5.3. The same workskation have been used to execute both the Model Trainer and the Link Evaluator components. As discussed later, the training and evaluation speed have been bottlenecked by the available single core performance of the CPU and by the amount of GPU memory.

Table 5.3: Hardware and software specifications of the workstation used to run the Model Trainer and the Link Evaluator.

Workstation hardware and software specifications	
CPU	x86-based with 4 cores and 8 threads clocked at 3.9GHz.
System memory	32GB of DDR3 1600MHz RAM.
GPU	8GB of VRAM and 2304 cores.
Boot drive	512GB SATA-III solid state drive.
Swap memory	A dedicated 64GB partition on the boot drive.
OS	Ubuntu Server 18.04 LTS with Linux Kernel 4.15.
SW packages	CUDA toolkit 10.1, Python 3.7.4, PyTorch 1.2 and DGL 0.3.

As saw in the previous section, the input dataset for the Model Trainer is composed by a list of edges, where 90% of them are used for the training, and the remaining are splitted in half and used for the validation and testing of the model. The training edges are used to build a *training graph*, which is the one that will be used to learn the node embeddings. Regarding the node features, a featureless approach has been followed, leveraging only the graph structure to learn the embeddings. Following this approach, the input features used are one-hot encoded vectors, thus obtaining an $N \times N$ feature matrix, where N is the number of nodes in the training graph.

Regarding the architecture, an R-GCN composed of two hidden layers has been employed, with the first layer convolutional filters being $500 \times N$, and the second layer filters being 500×500 . With such architecture the embeddings obtained as output of the forward pass are shaped as 1×500 row vectors. For the input layer, the one-hot encoded feature vectors

simply act as a mask for the selection of the corresponding column in the per-relation convolutional filters. Regarding the per-node normalization constants, they are initialized to the inverse of the nodes indegree.

Because of the size of the graph, and of the system memory available, the training is performed in batches. To do so, at each training epoch the Model Trainer randomly samples a subset of the training edges. As a consequence of this, more than one epoch is required to train over all the nodes in the training graph.

After the edges have been sampled, a predefined number of corrupted edges are generated starting from the sampled ones. This is done because the learning problem that has to be solved is a classification problem: the model has to be able to give a high score to the true edges, and a low score to the corrupted ones. This will allow to obtain a model that is able to recognize true facts, and thus can be used to predict the probability with which an unseen triple may belong to the Polito Knowledge Graph.

The negative samples are obtained by corrupting the subject and the object of the sampled training triples with a random integer. Such random integer must never assume a value equal to the index of a node. This is mandatory to avoid that within the negative samples there are triples that could be correct with respect to the ontology, and thus could be predicted by the Link Evaluator as new facts. Moreover, if the above condition is not met, some of the corrupted negative samples could be referring to facts that are actually true, thus interfering with the learning process.

The positive samples (the true facts) are associated to the label 1, while the negative samples are associated to the label 0. A 1-to-10 ratio has been chosen for the negative samples, having ten corrupted edges generated starting from each true fact, as it is done for most models found in literature that leverages negative sampling.

The embeddings of the relations are randomly initialized and not learnt by the model, as already mentioned when introducing the DistMult factorization method in section 2.2.3.

At each epoch the model is trained by performing the following steps:

1. The forward pass of the R-GCN is executed, taking as input the *DGLGraph* generated starting from the positive samples (the sampled training edges), which contains both the nodes features and the per-edge normalization constants. The neural network gives as output

the embeddings of the graph nodes.

2. Such embeddings are used to calculate the DistMult scores of both the positive and the negative samples. The sigmoid⁵ function is used to cap the scores between zero and one. Such capped scores represents the probabilities with which the model considers the corresponding edges as true facts.
3. The batch loss is calculated and the filters parameters are updated through backpropagation using the Adam [23] optimizer.

The loss function used is the *binary cross entropy loss* with mean reduction, which is commonly used for classification tasks with just two classes:

$$\mathcal{L}(x, y, f(x)) = -\frac{1}{E} \sum_{i=1}^E (y_i \cdot \log(f(x_i)) + (1 - y_i) \cdot \log(1 - f(x_i))) \quad (5.1)$$

E is the number of edges for the current batch, taking into account both positives and negatives samples, and y_i represents their associated label.

The function $f(x_i)$ computes the predicted probability for the i -th sample to be a true fact by applying the sigmoid function to its score, which is calculated with the DistMult factorization method:

$$f(x_i) = f(s_i, r_i, o_i) = \sigma(e_s^T R_r e_o) \quad (5.2)$$

Where e_s and e_o are the embeddings for the source node (subject) and destination node (object), R_r is obtained by transforming the embedding of the relation e_r into a diagonal matrix and σ is the sigmoid function. The resulting value can be interpreted as the confidence of the model in the fact that the corresponding edge represents a true fact.

The loss function used sets as training goal the correct classification of negative and positive samples, so to obtain a score as low as possible for the negative ones, while instead identify the true triples sampled from the PKG as true facts, thus giving them an high score.

⁵ $\sigma(x) = \frac{1}{1+\exp^{-x}}$

As a consequence of this, the obtained model should be able to correctly predict if an unseen triple can be considered as a good candidate for the inclusion in the Polito Knowledge Graph.

To avoid overfitting, the following $L2$ regularization is added to the training loss:

$$regularization = \lambda \cdot \left(\frac{1}{N} \sum_{i=0}^N e_i^2 + \frac{1}{R} \sum_{r=0}^R w_r^2 \right) \quad (5.3)$$

Where λ is an hyperparameter used to scale the regularization value, N is the number of nodes, R is the number of relations, e_i is the embedding of the i -th node and w_r is the already mentioned randomly initialized vector that represents the embedding of the relation r .

In addition to the regularization, dropout with a probability of 20% is used to randomly update only some of the network weights at each training epoch.

The training can be performed both on CPU, which in respect to the GPU has access to four times the memory, but has less execution units, or on the GPU, which is memory-limited but can leverage its highly parallelized architecture. The usage of CPU or GPU and the number of CPU threads to be used are hyperparameters that can be chosen in advance, before starting the training.

The training has been performed on GPU with a sampling size of 20,000 edges, that adding the negative samples produces a per-epoch training set composed of a total of 220,000 edges. Perform the training over more edges was not feasible with the only 8GB of VRAM available. While having to train over more epochs due to the video memory constraints, in comparison to the execution on the CPU the training time has been reduced by two order of magnitude: from approximately 30 seconds per epoch for the forward plus backward pass, to less than 0.3.

The biggest bottleneck while training remains the sampling phase, which is implemented as single threaded code using NumPy [24], and requires approximately five seconds to be performed with the hardware at our disposal, which has fairly limited single-threaded performances. The implementation of more efficient sampling methods is leaved for future releases.

In order to identify the best parameters, the model has been evaluated on a separate validation set during training. The validation is not performed at every epoch due to computation time constraints, and the

frequency with which it is executed is an hyperparameter of the model. The evaluation method and the metrics used to test the accuracy of the trained model will be presented in the next chapter. If during the validation the model trained at the current epoch is identified as the best so far, its parameters are serialized and locally stored. Once the training is finished, the previously exported best epoch model is loaded from memory and its accuracy is evaluated on the test set.

After the training, validation and test phases are completed, the obtained encoder model should be able to give as output meaningful embeddings of the PKG nodes, which can be used to evaluate new facts using a factorization method like DistMult as decoder.

5.2.3 The Link Evaluator

Once the model has been trained, and the testing phase showed that it has embedded the characteristics needed to build semantically meaningful nodes embeddings, the Link Evaluator can be used to leverage the trained model for the prediction of new facts.

As already saw, a *fact* in the knowledge base is composed of a source and a destination node, the subject and the object, and a relation, called predicate, that connects the two nodes establishing a connection between them.

The goal of the Link Evaluator is the prediction of facts that are not already present in the knowledge base, and that are coherent with the defined ontology, both in domain (for the subject) and range (for the object).

The Link Evaluator loads in memory the model produced by the Model Trainer and performs the following tasks:

1. It builds the graph of existing facts by merging together the train, test, and evaluation edges.
2. Then, it gets the embeddings of the nodes of such graph by feeding it to the trained encoder.
3. It creates the set of every possible fact and it scores the triples in such set, only taking the ones with the highest score.
4. Finally, the obtained predicted triples are saved in a JSON file and imported by the Graph Builder, that will add them to the Polito Knowledge Graph as new RDF statements.

The node embeddings are obtained by feeding the graph of existing facts to the R-GCN encoder in evaluation mode, so to disable the gradients tracking in the PyTorch computational graph, which greatly improves the performances.

To create the set of new facts, the Link Evaluator firstly generates the set of all the graph nodes, and then creates the set of possible facts by generating, for every node, all the possible links to every other node in the graph. This is done by taking for each source node (subject) all the possible permutations of relations (predicates) and destination nodes (objects).

However, the majority of such automatically generated triples will be semantically incorrect. For example, among the permutations there will be triples that connect together two publications using as predicate the relation *dc:subject*, which is clearly meaningless, because it is saying that the major topic of a publication is another publication. For this reason, the triples that are not correct with respect to the PKG ontology are immediately discarded.

Once the semantically incorrect facts are removed, the remaining edges could be scored by applying the DistMult factorization. Then, the scored triples are grouped by subject and relation and sorted by their score in descending order. The number of scored triple to save for each couple subject-relation is an hyperparameter decided in advance, with 30 being the default value. The resulting new facts are then exported as a JSON file that can be used by the graph builder to create the corresponding RDF triples. Such triples can then be added the Polito Knowledge Graph, completing its knowledge base with new facts.

Moreover, the predicted triples can be used to obtain insights and recommendations that can be shown by the Viewer module (which has been introduced in Chapter 3) in the search results. For instance, among all the predictions there will be triples that links researchers to publications that have been not authored by them: such predicted authors can be interpreted as researchers that shares the same research interests of the publication authors. Leveraging such predictions, the recommendation system can suggest unexplored research topics to the researchers, scientific journals that have published papers related to their field of research, or the profiles of other researchers who share the same research interest but with whome they have never worked before.

Chapter 6

Evaluation

In this chapter are described the methods adopted to evaluate the trained model. The evaluation phase is performed both during training and testing. For the training task, the evaluation of the model is done over the validation set, which is used to check whether the latest updated parameters led to a more accurate model. After the training is finished, the evaluation is performed over a test set whose data has never been seen by the model during training, so to test whether it is able to correctly score unseen true facts.

The model has been evaluated using the *entity ranking* approach, which is commonly used for the evaluation of knowledge base completion models. Such approach evaluates the ability of a model to identify the triples that belongs to the knowledge base with respect to the set of all possible facts.

To do so, it is firstly required to generate two sets of perturbed facts for each triple inside the knowledge base. This is actually performed by perturbing the source and destination node of every edge in the evaluation set with all the possible entities that compose the graph.

Doing so, starting from the i -th evaluation edge (s_i, p_i, o_i) two sets of perturbed edges (a, p_i, o_i) and (s_i, p_i, b) are obtained, with $a, b \in [0, N]$, where N is the number of nodes in the graph.

Then, for every triple in the evaluation set, the triple itself and its corresponding perturbed ones are scored using the same factorization method used for the training, in this case DistMult. The triples are then sorted in descending score, and the position of the evaluation triples inside such sorted list represent their *rank*.

Ideally, the best possible model should be able to always rank all the

triples in the evaluation set on first position, thus giving them the highest rank, which is equal to 1. Such model would be always able to identify the correct facts, and therefore one could be confident in the truthfulness of its predictions. However, obtaining such model is unfeasible.

To obtain a measure of the accuracy with which the trained model is able to identify the correct triples, the following metrics have been used:

1. The Reciprocal Rank (RR), which can be computed for a single evaluated edge (s_i, p_i, o_i) as $1/\text{rank}_{(s_i, p_i, o_i)}$, where the rank is obtained as explained above.
2. The Mean Reciprocal Rank (MRR), which is the average of the RR of all the evaluation edges. The value obtained is representative of the accuracy of the entire model.
3. The Hits-at-N (HITS@N), which is the number of triples for whom the computed rank is between 0 and N .

So for example, a triple ranked in the tenth position of the sorted list of scores will have a RR of 0.1. If the triples in the evaluation set are 100, with half of them ranked in first position and the other half in the tenth, the obtained MRR will be $\frac{1}{100} \sum_{i=1}^{100} \frac{1}{\text{rank}_{(s_i, r_i, o_i)}} = 0.55$, while the HITS@1 will be equal to 50, and the HITS@10 will be equal to 100.

The evaluation has been performed on the same workstation used for the training, whose specifications can be found in Table 5.3. However, in contrast to the training, which is performed on GPU to leverage its parallelized architecture, the evaluation had to be made on CPU due to memory constraints. This because, as a consequence of the dimensionality of the graph, and therefore that of the set of perturbed edges, the matrices used to perform the evaluation cannot be stored in the GPU memory. Moreover, also the system memory available was not sufficient to perform such task in parallel for all the edges, thus requiring the evaluation to be performed in batches. With the system memory available in the workstation, it has been possible to perform the evaluation in batches of 80 triples.

Because of the above limitations, the evaluation proved to be the slowest task of the whole pipeline, taking approximately twenty minutes per run. This is the main reason why it has been not possible to perform the evaluation of the model at every training epoch. However, evaluating the

Table 6.1: Evaluation of different combinations of learning rate and regularization parameters using as benchmark the MRR value. The first table shows the MRR of the best model found during the training phase. The second table shows the MRR obtained by the best model over the test set.

(a) MRR of the best model found during training.

		Learning Rate				
Regularization	MRR	0.05	0.01	0.005	0.001	0.0005
	1.0		0.0623	0.0504	0.0823	0.0793
	0.5		0.0677	0.0718	0.0924	0.0865
	0.1	0.0004	0.0703	0.852	0.0764	0.0706
	0.05		0.0707	0.0763	0.0673	
	0.01		0.062	0.0725		

(b) MRR obtained when evaluating the best model over the test set.

		Learning Rate				
Regularization	MRR	0.05	0.01	0.005	0.001	0.0005
	1.0		0.0611	0.0497	0.081	0.079
	0.5		0.0662	0.0723	0.0882	0.0818
	0.1	0.0002	0.0693	0.0827	0.0726	0.0666
	0.05		0.0687	0.0726	0.0654	
	0.01		0.0589	0.07		

trained model every 100 epochs still allowed to obtain useful metrics for the choice of the best hyperparameters.

In Table 6.1 are shown the results of the evaluation of the model over some possible values of the hyperparameters, in particular, the MRR for possible combinations of the learning rate and of the regularization parameter has been calculated. As can be saw from the table, the best

values found are 0.001 for the learning rate and 0.5 for the regularization parameter.

The high value of the regularization parameter, if compared to the one used by the R-GCN authors (which is 0.01), is particularly interesting: the motivation of this result is that the Polito Knowledge Graph, and thus the training graph used, is composed of a very low number of different relations, which is particularly true if compared to other graphs, such as the one used for benchmarking. Given how the R-GCN encoder works, less relations means less convolutional filters, so less variety in the features that are used to generate the embeddings. In this regard, the regularization parameter helps the model to differentiate the embeddings obtained, even if there are few relations, and allows to not overfit on common features.

Regarding the MRR value obtained for the best model, it can be interpreted as the fact that, in average, the evaluated triples are ranked in the *eleventh* position. The authors of R-GCN obtained an MRR value of 0.158 over the FB15k-237 dataset (composed of 14,541 entities and 237 different relations), which is commonly used as benchmark for the evaluation of link prediction model. The MRR obtained by the authors correspond to a ranking that, in average, place the evaluation triples in the sixth or seventh position. The result obtained is thus not so distant from the one obtained over the benchmarking dataset.

Moreover, considering the number of nodes in the PKG dataset, the result obtained is particularly noteworthy, given that the model is able to rank (in average) the true triple in the eleventh position when ranked with 47,995 corrupted triples, while in FB15k-237 for each true fact only 14,951 corrupted ones are generated.

The Figure 6.1 shows how the testing triples are distributed over the possible ranking values. As can be saw, the model is able to correctly assign an high rank to the majority of the true facts.

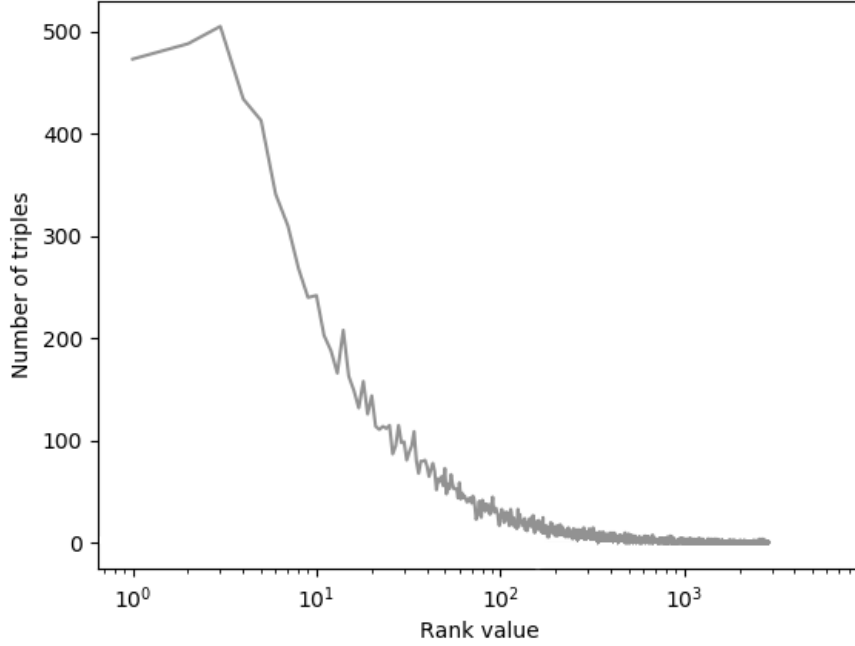


Figure 6.1: Number of triples for each ranking position obtained by evaluating the best model found over the test set. The ranking positions range from 1 to 47,995.

When looking at the statistics of the Polito Knowledge Graph, it is possible to see how a large part of the entities are related to the research topics, represented by the *TMFResource* instances, and connected to the publications by means of the *dc:subject* relation. In particular, as shown in Table 5.1, almost a third of the PKG edges link a publication to a subject extracted by TellMeFirst.

To evaluate the impact of having a different number of *TMFResource* entities in the knowledge graph three new RDF graphs have been built, each of them with a different number of topics extracted by TellMeFirst for each publication. In particular, have been extracted three, seven and fourteen topics from each abstract. Then, the corresponding models have been trained by giving as input the datasets created starting from such new graphs. For the learning rate and the regularization hyperparameters, the best values found during the previous evaluation have been used.

As can be seen from the results shown in Table 6.2, the different number of topics present in the three graphs greatly impact in the accuracy of the resulting link prediction models.

Table 6.2: Impact of the number of topics present in the RDF graph on the accuracy of the trained model.

Number of topics extracted per-abstract	3	7	14
Number of <i>TMFResource</i> entities in the graph	9.591	16.988	26.541
Number of <i>dc:subject</i> edges	45.423	107.093	212.226
MRR over test data	0.103	0.0882	0.0671
HITS@15	31.5%	27.9%	20.3%

Lowering the number of topics extracted to just three for each publication resulted in an improvement in the evaluation metrics, however, this did not lead to a better link prediction model. In fact, the better ranking is a consequence of the less complex graph structure: being the graph composed of almost half of the topic entities, is more simple for the model to rank in a higher position the evaluated triples. Moreover, there are more publications that shares the same topics, thus leading to a model that is very capable of predicting the triples corresponding to such topics as true facts during the evaluation over the test set.

Instead, increasing the number of topics inside the graph led to a degradation of the evaluation metrics. This can be easily be interpreted as a consequence of the more complex graph structure obtained. Moreover, the increase in the number of *dc:subject* edges may have led to a predominance of the topics when encoding the neighborhood representations through the R-GCN, thus bringing a bias in the nodes embeddings obtained. This could then impact on the results of the decoder, thus bringing to more inaccurate predictions.

As already mentioned in the previous Chapter, the predicted triples are saved in the form of a JSON file that is then used to load the new facts in the knowledge base. The predicted triples are the ones that received the highest score by the DistMult decoder, thus being recognized as facts that, with an high likelihood, should belong to the knowledge base.

A manual and sample-based validation confirmed that the model obtained has been able to truly characterize the graph entities, thus predicting meaningful triples. For example, the model predicted for a publication regarding real-time tools for emergency management a new *dc:subject* edge

that links such publication to a DBpedia resource¹ which collects the list of software reliability models, which looks like an appropriate suggestion. The model also predicted a new edge that connects the above publication to a researcher whose main field of research is in integrated circuits for aircraft applications, which is again a good prediction being the two topics fairly related. The above examples are just two among all the new, meaningful facts that the model has been able to predict. However, it is also true that there are predictions which are not correct, in particular the ones regarding researchers who have a very low amount of publications, for example students in their first years of PhD, or the ones of publications that have a very misunderstandable abstracts, thus leading to an incorrect topic extraction by TMF. Some possible solutions to such issues are proposed in the next Chapter, where are presented the possible future developments in this regard.

¹Entity URI: http://dbpedia.org/resource/List_of_software_reliability_models

Chapter 7

Conclusions and Future Work

In this work has been presented a new academic Knowledge Graph built on top of the metadata of the Politecnico di Torino publications. Such knowledge graph links together researchers, publications, research topics and scientific journals through the use of semantic relations.

The software architecture developed for the creation, enhancement and visualization of such graph has been detailed, particularly focusing on the enhancing phase. In this regard, an approach based on Graph Convolutional Networks has been used, so to obtain an encoder model capable of embedding the nodes characteristics into vector representations by only taking the graph structure as input. Such representations allowed to predict new facts, so to complete the information available in the knowledge base. Such predicted facts have been used to empower a recommendation system whose suggestions can be used by the researchers to explore new fields of study, to discover other researchers who share the same research interests or for retrieving other useful insights about their scientific community.

The scholarly data of any other academic institution could be used to build a similar graph. Moreover, metadata coming from different universities can be grouped together to obtain a bigger and more complete knowledge graph, representative of an even broader academic community. With this regard, I look forward to obtain the metadata of other universities who employ IRIS as their publications repository.

Regarding the technological aspects, I would like in future releases to

implement new factorization methods, testing whether or not the use of different scoring functions can lead to even more accurate link prediction models. Moreover, one of the main limitations of the current implementation of the Enhancer Module is that it is not able to predict new facts regarding entities that the model has never seen during training. I would like to investigate in this regard for new solutions based on the extension of the current encoder architecture. I would also like to test the use of input features generated using a bag-of-words approach instead of the simple one-hot encoded vectors used for the current model.

Another aspect that could be improved is the structure of the graph itself. In the current implementation there are no dependencies or relations between the research topics entities, however, this could be implemented in future releases by linking together the topics based on how they are related to each other. For example, *Deep Learning* is a sub topic of *Machine Learning*, which in turn is a sub topic of *Artificial Intelligence*, but at the time of writing this kind of information is not present in the Polito Knowledge Graph. Such improvement could be achieved by leveraging the structured information made available by the DBpedia project. Moreover, the Dataset Builder could leverage such new information, keeping only the specialized topics and discarding the most general ones. This could help to obtain more characterized embeddings, as already discussed in the previous chapter.

Moreover, an important aspect would be to collect some feedbacks from researchers, who are the main users for whom this tool has been designed. Such feedbacks could be used to introduce a bias during the training phase, so to penalize possible incorrect facts that have been wrongly predicted by the Link Evaluator.

This work has shown how is it possible to build new tools for the sharing and dissemination of the knowledge produced by an academic institution leveraging technologies of the Semantic Web and state-of-the-art machine learning algorithms. The recommendation system is a first step in the direction of offering new tools to the researchers for exploring both new research fields and the scientific community that study such fields. Hopefully, this could lead to the contamination between researchers belonging to different research areas but that are interested in the same research topics, thus increasing the multidisciplinary within the Politecnico di Torino academic community.

Moreover, the Polito Knowledge Graph and its recommendation system can be also used by administration offices of the Polito di Torino and from external parties – such as private organizations or government agencies – who may be interested in finding expert profiles in a given research area, breaking the current silos of keyword-based searches or discipline-specific knowledge bases.

Bibliography

- [1] Y. G. Natasha Noy, A. N. Anshu Jain, and J. T. Alan Patterson, “Industry-scale knowledge graphs: Lessons and challenges,” *Communications of the ACM*, vol. 62, no. 8, pp. 36–43, 2019. [Online]. Available: <https://cacm.acm.org/magazines/2019/8/238342-industry-scale-knowledge-graphs/fulltext>
- [2] M. Schlichtkrull, T. N. Kipf, P. Bloem, R. Van Den Berg, I. Titov, and M. Welling, “Modeling relational data with graph convolutional networks,” in *European Semantic Web Conference*. Springer, 2018, pp. 593–607. [Online]. Available: https://link.springer.com/content/pdf/10.1007%2F978-3-319-93417-4_38.pdf
- [3] L. Page, S. Brin, R. Motwani, and T. Winograd, “The pagerank citation ranking: Bringing order to the web.” Stanford InfoLab, Technical Report 1999-66, November 1999, previous number = SIDL-WP-1999-0120. [Online]. Available: <http://ilpubs.stanford.edu:8090/422/1/1999-66.pdf>
- [4] D. L. McGuinness, F. Van Harmelen *et al.*, “Owl web ontology language overview,” W3C recommendation, Tech. Rep., 2004. [Online]. Available: <https://www.w3.org/TR/2004/REC-owl-features-20040210/>
- [5] O. Lassila and R. R. Swick, “Resource description framework (rdf) model and syntax specification,” W3C recommendation, Tech. Rep., 1999. [Online]. Available: <http://www.w3.org/TR/1999/REC-rdf-syntax-19990222/>
- [6] B. DuCharme, *Learning SPARQL: querying and updating with SPARQL 1.1*. "O'Reilly Media, Inc.", 2013.
- [7] M. Graves, A. Constabaris, and D. Brickley, “Foaf: Connecting people on the semantic web,” *Cataloging & Classification Quarterly*, vol. 43, no. 3-4, pp. 191–202, 2007. [Online]. Available: <https://>

[//doi.org/10.1300/J104v43n03_10](https://doi.org/10.1300/J104v43n03_10)

- [8] S. Weibel, J. Kunze, C. Lagoze, and M. Wolf, “Dublin core metadata for resource discovery,” *Internet Engineering Task Force RFC*, vol. 2413, no. 222, p. 132, 1998. [Online]. Available: <http://www.hjp.at/doc/rfc/rfc2413.html>
- [9] T. Mikolov, K. Chen, G. Corrado, and J. Dean, “Efficient Estimation of Word Representations in Vector Space,” *arXiv e-prints*, p. arXiv:1301.3781, Jan 2013, provided by the SAO/NASA Astrophysics Data System. [Online]. Available: <https://arxiv.org/pdf/1301.3781.pdf>
- [10] T. N. Kipf and M. Welling, “Semi-Supervised Classification with Graph Convolutional Networks,” *arXiv e-prints*, p. arXiv:1609.02907, Sep 2016, provided by the SAO/NASA Astrophysics Data System. [Online]. Available: <https://arxiv.org/pdf/1609.02907.pdf>
- [11] A. Krizhevsky, I. Sutskever, and G. E. Hinton, “Imagenet classification with deep convolutional neural networks,” in *Advances in neural information processing systems*, 2012, pp. 1097–1105. [Online]. Available: <http://papers.nips.cc/paper/4824-imagenet-classification-with-deep-convolutional-neural-networks.pdf>
- [12] J. Gilmer, S. S. Schoenholz, P. F. Riley, O. Vinyals, and G. E. Dahl, “Neural message passing for quantum chemistry,” in *Proceedings of the 34th International Conference on Machine Learning-Volume 70*. JMLR. org, 2017, pp. 1263–1272. [Online]. Available: <https://arxiv.org/pdf/1704.01212.pdf>
- [13] B. Yang, W.-t. Yih, X. He, J. Gao, and L. Deng, “Embedding entities and relations for learning and inference in knowledge bases,” *arXiv preprint arXiv:1412.6575*, 2014. [Online]. Available: <https://arxiv.org/pdf/1412.6575.pdf>
- [14] O. R. Rocha, I. Vagliano, C. Figueroa, F. Cairo, G. Futia, C. A. Licciardi, M. Marengo, and F. Morando, “Semantic annotation and classification in practice,” *IT Professional*, vol. 17, no. 2, pp. 33–39, Mar 2015.
- [15] P. Cifariello, P. Ferragina, and M. Ponza, “Wiser: A semantic approach for expert finding in academia based on entity linking,” *Information Systems*, vol. 82, pp. 1–16, 2019. [Online]. Available: <https://arxiv.org/pdf/1805.03947.pdf>
- [16] A. Salatino, F. Osborne, T. Thanapalasingam, and E. Motta,

- “The cso classifier: Ontology-driven detection of research topics in scholarly articles,” *TPDL 2019: 23rd International Conference on Theory and Practice of Digital Libraries*, 2019. [Online]. Available: <http://oro.open.ac.uk/62026/>
- [17] M. Defferrard, X. Bresson, and P. Vandergheynst, “Convolutional neural networks on graphs with fast localized spectral filtering,” in *Advances in neural information processing systems*, 2016, pp. 3844–3852. [Online]. Available: <http://papers.nips.cc/paper/6081-convolutional-neural-networks-on-graphs-with-fast-localized-spectral-filtering.pdf>
- [18] D. K. Duvenaud, D. Maclaurin, J. Iparraguirre, R. Bombarell, T. Hirzel, A. Aspuru-Guzik, and R. P. Adams, “Convolutional networks on graphs for learning molecular fingerprints,” in *Advances in neural information processing systems*, 2015, pp. 2224–2232. [Online]. Available: <https://papers.nips.cc/paper/5954-convolutional-networks-on-graphs-for-learning-molecular-fingerprints.pdf>
- [19] S. M. Kazemi and D. Poole, “Simple embedding for link prediction in knowledge graphs,” in *Advances in Neural Information Processing Systems*, 2018, pp. 4284–4295. [Online]. Available: <http://papers.nips.cc/paper/7682-simple-embedding-for-link-prediction-in-knowledge-graphs.pdf>
- [20] T. Trouillon, J. Welbl, S. Riedel, É. Gaussier, and G. Bouchard, “Complex embeddings for simple link prediction,” in *International Conference on Machine Learning*, 2016, pp. 2071–2080. [Online]. Available: <http://proceedings.mlr.press/v48/trouillon16.pdf>
- [21] A. Paszke, S. Gross, S. Chintala, G. Chanan, E. Yang, Z. DeVito, Z. Lin, A. Desmaison, L. Antiga, and A. Lerer, “Automatic differentiation in pytorch,” *NIPS 2017 Workshop Autodiff Submission*, 2017. [Online]. Available: <https://openreview.net/pdf?id=BJJsrnfCZ>
- [22] M. Wang, L. Yu, D. Zheng, Q. Gan, Y. Gai, Z. Ye, M. Li, J. Zhou, Q. Huang, C. Ma *et al.*, “Deep graph library: Towards efficient and scalable deep learning on graphs,” *arXiv preprint arXiv:1909.01315*, 2019. [Online]. Available: <https://arxiv.org/pdf/1909.01315.pdf>
- [23] D. P. Kingma and J. Ba, “Adam: A method for stochastic optimization,” *arXiv preprint arXiv:1412.6980*, 2014.
- [24] T. E. Oliphant, *A guide to NumPy*. Trelgol Publishing USA, 2006, vol. 1.