

POLITECNICO DI TORINO

DEPARTMENT OF CONTROL AND COMPUTER ENGINEERING

Master of Science in Computer Engineering

Master Degree Thesis

Deep Learning on Polito Knowledge Graph

Leveraging Relational GCN for link prediction between nodes of
a newly built publications graph



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ACADEMIC YEAR 2018-2019

To Monia

To my Grandfather

Abstract

Summary here, one page

Acknowledgements

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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 engine ¹. They 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. RDF graphs are a particular class of graphs that can be used to build knowledge bases. 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 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, so as not to require any feature engineering.

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

1.2 Goal and contribution

Today scholarly data can be accessed through web portals that allow to retrieve scientific papers published by researchers. One example is the IRIS portal², that stores all the publications of the Turin Polytechnic University researchers. IRIS allow to retrieve publications by field of interest, matching the user input with the keywords inserted by the author. The current implementation has some main limitations: ambiguity may arise, having papers that deals with the same subject represented by different keywords, or having acronyms or misspelled keywords that refer to the same argument. The system is thus not able to search for *semantic concepts*, but only for a character string that is matched against the keywords available in the database, which are not unique and prone to lexical error.

Building a new semantic empowered search engine can be one of the possible solutions to overcome such limitations, 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 by automatically extracting latent information through the use of advanced machine learning algorithms.

In the next chapters we are going to present a newly built structured and semantically coherent representation of the scholarly data produced by the Turin Polytechnic University, and how implicit facts can be automatically extracted from such knowledge repository by leveraging knowledge base completion techniques, implemented by means of an advanced deep learning algorithm.

1.3 Thesis structure

1.3.1 Chapter 2

1.3.2 Chapter 3

1.3.3 Chapter 4

²<https://iris.polito.it/>

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: we can think of documents as nodes and hyperlinks as edges. The unstoppable growth of the *Web graph* led to the raise of new tools to extricate in such complexity. Search engines have been developed to easily navigate such a giant graph, initially by scoring search results based on trivial statistics, such as the number of times a document has been linked, as in the case of the PageRank [2] 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 Graph ¹, 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
2. RDF: the Resource Description Framework
3. SPARQL: The SPARQL Protocol and RDF Query Language

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.

RDF is a XML-based framework that 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 vocabularies have been built on top of RDFS, such as the Friend of a Friend (FOAF) vocabulary [3], for describing social networks, or the one maintained by the Dublin Core Metadata Initiative [4], that defines common terms used in the definition of metadata for digital resources.

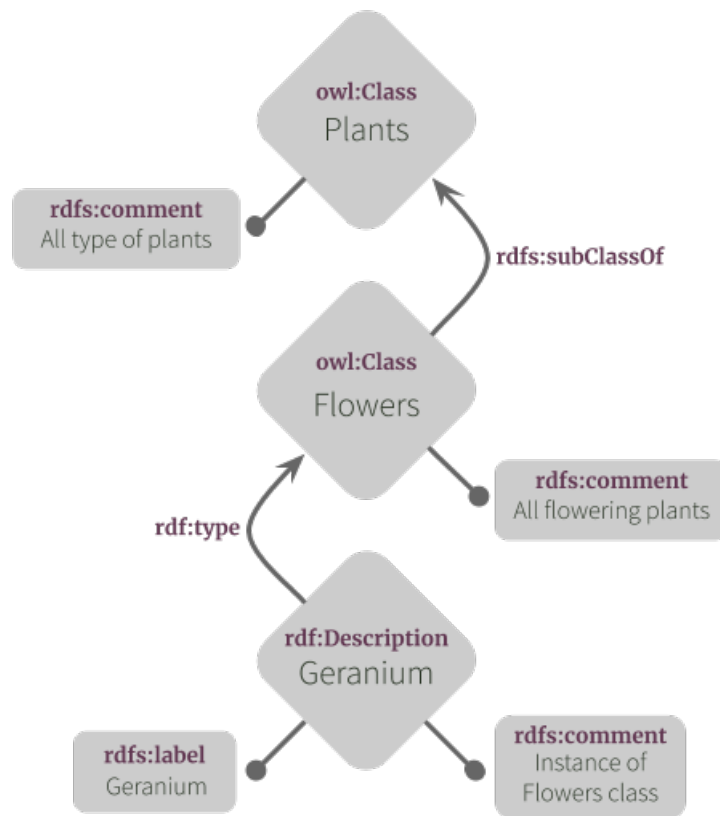


Figure 2.1. An example of ontology defined using OWL and RDF Schema.

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 data stored, the query language has been designed to be as simple as possible, in example 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 if 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 unstructured 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 contains, describes and links more then three hundred million academic papers.

From an implementation perspective, knowledge bases can be created

²<https://wiki.dbpedia.org/>

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

⁴<https://www.openacademic.ai/oag/>

to describe a specific domain by defining an ontology and a vocabulary for such domain 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 biggest effort when building knowledge bases is to have a correct understanding and prior knowledge of the domain of interest, to avoid the risk of mischaracterizing and misrepresenting concepts.

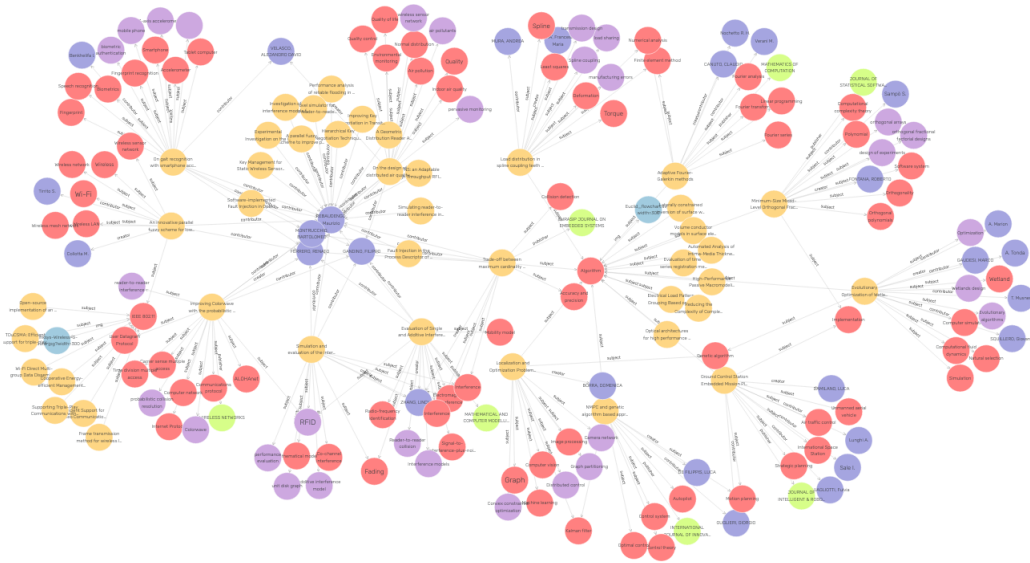


Figure 2.2. An extract of the Polito Knowledge Graph that will be introduced and described in the following chapters.

If all the requirements and cautions are met, a well formed knowledge base may prove to be a critical resource for an organization. It allows not only to build new services upon it, but also to improve the existing knowledge inside the organization by performing reasoning upon the available knowledge, thus to discover implicit facts that can be derived from existing relationships. Another field of applications is the development of Expert Systems, 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 by tens of thousands nodes and by hundreds of thousands of edges, such giant data structures pose many challenges. Not only storing and querying giant graphs requires

the adoption of specialized DBMS that are capable of efficiently store and query the RDF input representation, but also doing 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.

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 obtained models can be used to recognize unseen inputs by leveraging the knowledge embedded in such parameters. ML algorithms require the input data to be available in a machine-understandable vector representation. An important task in the ML field is the learning of such representations, task known as representation learning.

Natural Language Processing (NLP) 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 [5], 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're used in similar contexts, thus in the vector space of the learnt representations words that have similar meaning have higher cosine similarity⁵ with respect to dissimilar ones. For instance, the cosine similarity between the word vectors of "Man" and "King" is roughly

⁵ Cosine similarity is a heuristic method to measure the similarity between two vectors by computing the cosine of the angle between them: $similarity = \cos(\theta) = \frac{A \cdot B}{\|A\| \|B\|}$

the same as the one between the words "Woman" and "Queen", since such words are used in similar contexts. This has opened up new scenarios for language recognition and processing, since it allowed to perform vector operations on such words which brought interesting results, as can be seen in Figure 2.3.

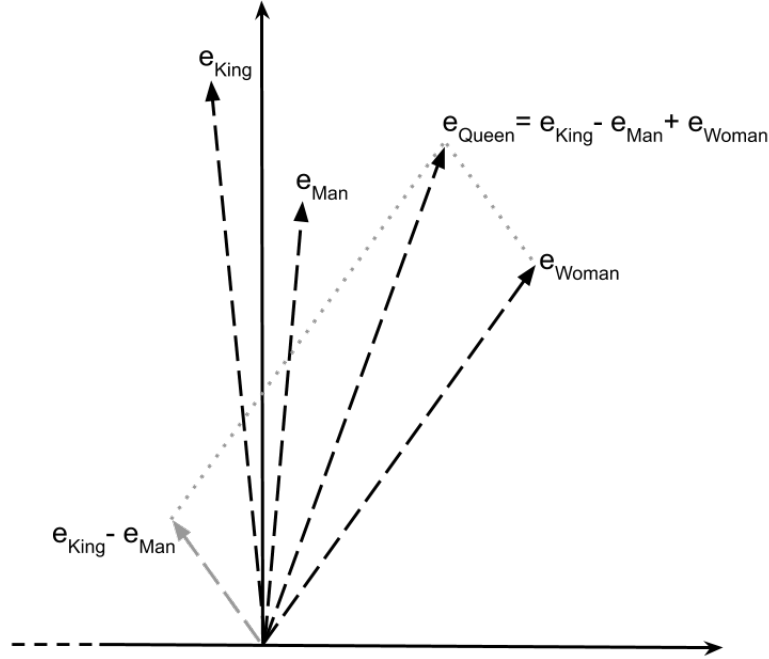


Figure 2.3. Word vectors allow to perform vector operations, the results obtained reflect the fact that Word2Vec is capable of embedding the meaning of such words.

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 by 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 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. In example, 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 (DL) 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 DL 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 by 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.

The issue of 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

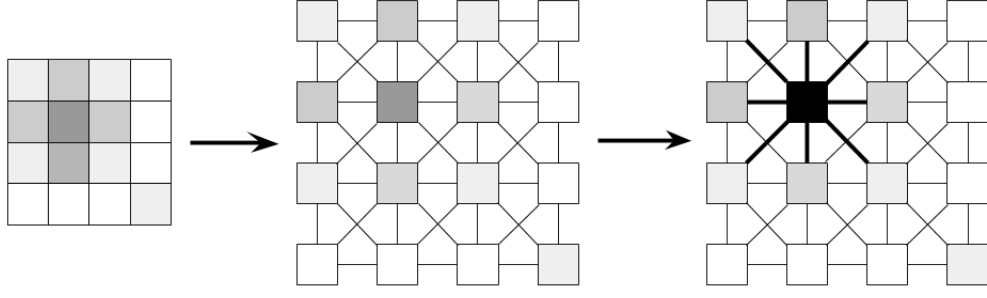


Figure 2.4. A digital image can be thought of as a graph.

sampling the graph at each training epoch, the immediate drawback being that more than one epoch is required to train over all nodes. The second issue can instead be solved by adapting known 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) [6] 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 (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 a convolutional filter, whose parameters are then updated during the backpropagation 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, this 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 is the output of the previous layer or, for the input layer, the node features matrix where each row is commonly initialized as a one-hot encoded feature vector. \tilde{A} is the adjacency matrix of the graph summed with the identity matrix to add self loops of nodes, \tilde{D} is the node degree matrix of \tilde{A} and is used to normalize it, W^l is the weight matrix of the layer, that is shared among all nodes for each layer, just like the

convolutional filter in a CNN, and $\sigma()$ is a non linear activation function, for example *ReLU*.

The forward rule to update the embedding of a single node at each layer of the network is the following:

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

Setting aside the normalization constant c_{ij} which is obtained from the multiplication between the adjacency and degree matrices, at each layer the updated feature vector of the node i is obtained by summing over all the nodes in its neighborhood the result of the multiplication between the neighbors feature vectors and the weight matrix of the layer. A consequences of applying this rule to all nodes is that at the l -th layer the feature vectors of nodes that are at a l hop distance from the node i will be embedded in its feature vector, because the feature vectors of such nodes were embedded, at the previous layer, by the immediate neighbors of node i , which are now passing the information of their surrounding to it. So the amount of layers of the network is a parameter that controls how much information from furthest nodes has to be collected by each node embedding.

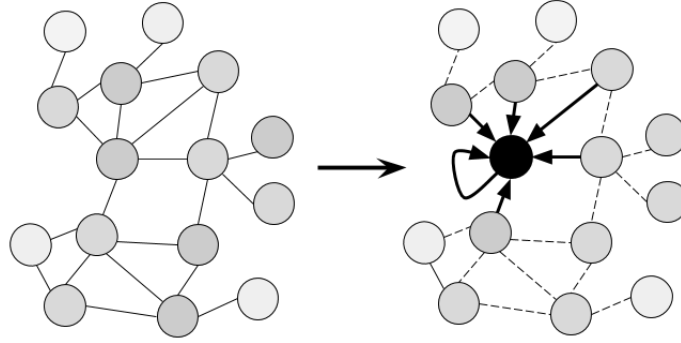


Figure 2.5. First layer of a GCN updating a node feature vector by embedding the features of adjacent nodes.

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, interests, places visited and so on, two people will have similar embeddings if they are connected to similar nodes.

The node embeddings obtained by applying a GCN or one of its variants can then be used to perform some learning task on the graph, two examples are the classification of unseen nodes or the link prediction of non-existent edges. The last example is one of the most interesting tasks because it empowers most of the recommendation systems available in the industry.

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 evaluate if unseen good candidates to be included in the knowledge base. Link prediction requires two main step:

1. Train an encoder model that is able to embed the node features and produce meaningful embeddings.
2. Apply a factorization model that is able 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 we use a single layer GCN to obtain the embeddings of two nodes that share the same neighborhood, but are connected to the neighbors via different relations, we'll obtain almost the same embeddings, even if it's 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 don't have the same role and don't 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.

Relational Graph Convolutional Networks [1] (R-GCNs) are an extension of GCNs that are focused on modeling multi-relational graphs composed by directed edges, and thus are particularly capable of embedding both nodes and relations of a knowledge graph. R-GCNs 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* [7], 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 by 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 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 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 is the embedding (or, for the first layer, the input feature vector) of the node i , W_0 is the learnt kernel for the relation between the node and itself (called self loop), \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 is the learnt kernel for the relation r . As for the GCN architecture, σ is a non linear activation function and $c_{i,j}$ 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 incoming edges of 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 parameters used to convolve the feature vectors of neighboring nodes are relation specific, this means that the kind of relation that connect the node to its neighbors has an important role in determining the node embedding.

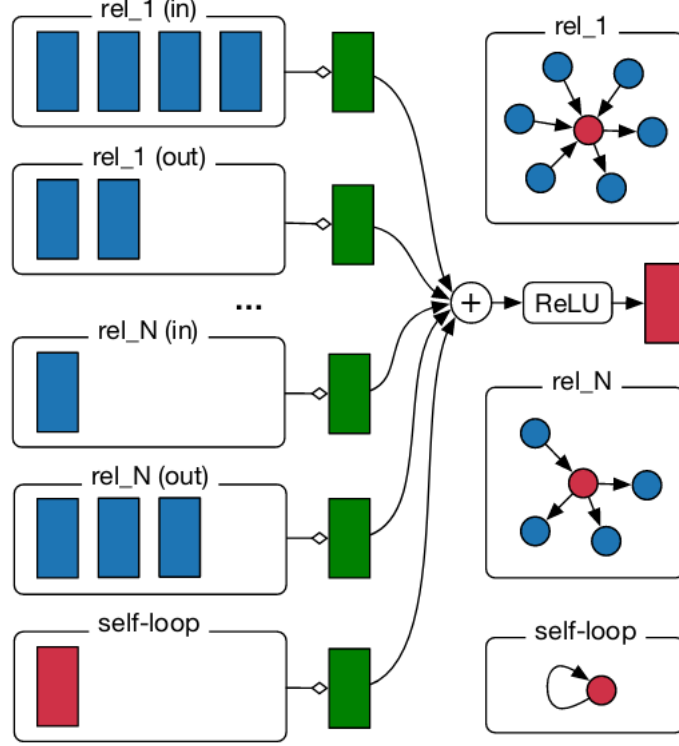


Figure 2.6. R-GCN encoder model. Image taken from [1].

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. One of the solutions proposed by the original paper [1] 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 an 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 [8] is one of the most common and simple factorization methods used to score unseen triples. Given as input the embeddings of the source node and destination node, and the relation parameter vector transformed into a diagonal matrix $R_r \in \mathbb{R}^{d \times d}$, it computes an associated real valued score:

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

The score obtained by applying such function 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 is to be interpreted as a high confidence of the model in the fact that the triple should belong to the knowledge graph.

Chapter 3

Approach and methodology

Chapter 4

Related work

Chapter 5

Development and implementation

5.0.1 Creating Polito Knowledge Graph

5.0.2 Training model on PKG

5.0.3 Link prediction on PKG

Chapter 6

Evaluation

Chapter 7

Conclusions and future work

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