Transformer-based knowledge graph completion

Uzupełnianie grafów wiedzy przy użyciu transformerów

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Abstract

Knowledge graphs play a crucial role in many systems used by billions of people, providing access to relations between various objects present in our daily life. In parallel, the knowledge contained in them is often incomplete. Therefore, the problem of completing knowledge graphs is becoming more and more important for humanity. The fact that most of them are very dynamic systems, makes it impossible for humans to fill out missing relations by hand. In the past, simple heuristic approaches have been tried to tackle the stated problem, but they covered only simple cases like inverse relations. With the rise of machine learning techniques, researchers started developing various model-based approaches, making tremendous progress over the past few years.

At this time, the most successful methods are based on convolutional neural networks, reinforcement learning and graph neural networks. In this thesis, we tackle the stated problem with transformer-based models, which have already found their applications in many sequence-to-sequence problems, outclassing other approaches. In particular, we develop a model operating on single edges as well as explore several approaches that add graph-based context to the model. Additionally, we compare the developed methods with other successful approaches on two popular benchmark datasets, called FB15K-237 and WN18RR.

Streszczenie

Grafy wiedzy odgrywają kluczową rolę w wielu systemach używanych przez miliardy ludzi, zapewniając dostęp do relacji między przeróżnymi obiektami obecnymi w naszym codziennym życiu. Jednocześnie, wiedza w nich zawarta jest często niepełna. Wynika stąd, że problem uzupełniania grafów wiedzy staje się coraz ważniejszy dla ludzkości. Fakt, że większość z nich to układy bardzo dynamiczne, uniemożliwia ludziom ręczne uzupełnianie brakujących relacji. W przeszłości próbowano prostych podejść heurystycznych do rozwiązania przedstawionego problemu, ale działały one tylko w prostych przypadkach, takich jak odwrotne relacje. Wraz z rozwojem technik uczenia maszynowego naukowcy zaczęli opracowywać różne podejścia oparte na modelach, osiągając ogromne postępy przez ostatnie kilka lat. Obecnie najlepsze metody opierają się na splotowych sieciach neuronowych, uczeniu ze wzmacnianiem i grafowych sieciach neuronowych.

W tej pracy podejmujemy postawiony problem przy pomocy modeli opartych na transformerach, które zdążyły już znaleźć swoje zastosowanie w wielu problemach mapowania sekwencji wejściowej do sekwencji wyjściowej, jednocześnie deklasując inne podejścia. W szczególności opracowujemy model operujący na pojedynczych krawędziach, a także badamy kilka podejść, które dodają do modelu kontekst oparty na grafie. Dodatkowo, porównujemy opracowane metody z innymi udanymi podejściami na dwóch popularnych zestawach danych, nazwanych FB15K-237 i WN18RR.

Contents

1. Introduction

In the following introductory chapter, we will define the notion of knowledge graph along with the problem of completing it. Furthermore, we will discuss the main motivations for solving the considered problem and give an overview of the past work. Finally, we will provide an outline of our approach to the problem of completing a knowledge graph.

1.1. Problem formulation

Consider a set of objects $e \in E$ and a set of relations between them $r \in R$. Formally, a **knowledge graph** is a set of triples $(e_1, r, e_2) \in K$, which represents relations between the considered objects. Particularly, $e_1 \in E$ is called to be in a (directed) relation $r \in R$ with $e_2 \in E$ if and only if $(e_1, r, e_2) \in K$. We will refer to an object $e \in E$ as an **entity** and to an object $r \in R$ as a **relation**. Besides it, when considering a triple (e_1, r, e_2), we will refer to e_1, e_2 as a **head entity** and a **tail entity**, respectively. In case one of entities in a given triple is missing, we will refer to it as a **target entity**, while the other entity that is known will be denoted as a **source entity**. From the practical perspective, we can think of our structure as a directed graph where vertices are represented by entities and edges are labelled by relations. A toy example illustrating a knowledge graph is shown in *Figure* 1.1.

While we would expect a knowledge graph to contain any information that is useful for a user, in practise the vast majority of relations are missing. This fact becomes intuitive when one realizes that adding one edge to a graph can add information about relations between several entities that are not adjacent to the added edge. As a result, the number of missing relations can grow exponentially with the increase of the number of edges. The problem of finding new relations in a knowledge graph is known as **Knowledge Graph Completion**.

Formally, we are given a knowledge graph G and our goal is to find triples $(e_1, r, e_2) \in K$ that are likely to represent true facts. Specifically, given a head entity $e_1 \in E$ and a relation $r \in R$, we aim to find a tail entity $e_2 \in E$, such that (e_1, r, e_2) is true. The analogous goal can be defined for a missing tail entity, given a head entity and a relation. The knowledge graph completion methods can be divided into those that extract information only from a graph and those that utilize additional information e.g. text-based definitions of entities. In this thesis, we only leverage information that is contained in a given graph, particularly our models falls into the graph-only category.

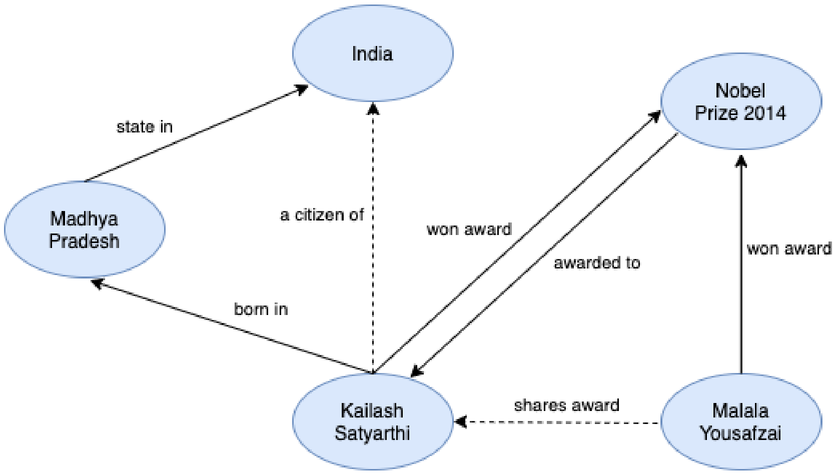


Figure 1.1: An example of a knowledge graph. Solid edges represent triples that are present in the knowledge graph, while dashed edges represent knowledge that is missing, but can be inferred directly from the graph.

1.2. Motivations for solving the problem

The first question to ask could be whether we really need a sophisticated model in order to complete a knowledge graph. Actually, most of knowledge graphs are very dynamic systems that evolve over time, making it impossible for humans to complete them by hand. Additionally, the problem of completing a knowledge graph is the very complex one. While simple heuristic approaches have been tried in the past, they only covered simple cases like inverse relations. As a result, in order to extract more sophisticated relations, we need a model that understands entities and their relations more deeply.

Solving the stated problem is motivated further by the fact that it has many real-world applications. First of all, consider a situation when you ask a voice assistant to answer a question about the nationality of your favourite actor. The answer to this question can be fetched from a knowledge graph, assuming that it is complete enough to contain this information. In order to be able to answer more questions, one needs to assure that the graph is complete. The class-leading voice assistants and search engines actually make use of knowledge graphs to provide answers to users' questions. Those graphs are developed by parsing online encyclopedias like

Wikipedia as well as news websites and as a result are often incomplete.

Knowledge graphs are are also useful in many other areas. For instance, they are used to boost recommendation engines of popular content and social media platforms. Furthermore, knowledge graphs are leveraged in the healthcare industry, enabling medical researchers to gain more insights from data. Additionally, they are also used to represent the relations between words in human languages. Lastly, knowledge graphs are leveraged by financial services to secure human decisions and prevent money laundering initiatives.

1.3. Related work

In the recent years, various approaches have been tried to tackle the problem of knowledge graph completion. The most successful ones are based on data-driven models, often called machine learning models. These methods will be discussed more deeply in the *Chapter* 2. For our task specifically, we can divide the considered models into ones that operate on triples alone (representing graph edges) i.e. context-free methods and those that utilize graph context e.g. neighbours of a head/tail entity. Recently, a new branch of models that leverage additional text-based information has been established, but those models are not considered in this thesis.

While the first context-free methods were proposed in 2013, the new models are still developed, surpassing the old ones. One of the first baseline models, learning latent representations of entities and relations, is known as the *TransE* model introduced in [1]. The model was later extended in [15] to *STranse*, which allows entities to have relation-specific representations. Several other improvements, utilising convolutional neural networks to learn better representations, have been proposed, including *ConvE* model presented in [19]. While many other context-free models have been developed, they retain the same quality of predictions. Therefore, we compare our methods only with the above-mentioned models.

In the past few years, several models have been developed to utilise context of a given graph. The first applications of those models to the considered problem have been proposed back in 2017. While many of the approaches failed to surpass context-free models, a few models have provided a considerable quality improvement. One of the successful approaches include [21] that tries to walk through a graph to find a matching entity. The other popular methods are based on graph neural networks, especially on the *GCN* architecture proposed in [23]. The best-performing ones include the *SACN* model presented in [22] and recently developed *CompGCN* model introduced in [29]. Although many other models have been proposed, as shown in [28], some of researchers have reported inflated quality results due to improper evaluation protocol. Therefore, we compare our models only with the models discussed above.

1.4. Our approach

One of the most ground-breaking machine learning architectures in the recent few years is the *Transformer* model introduced in [17]. It has been successfully applied to many sequence-to-sequence problems, outclassing other models. Moreover, several improvements have been proposed to the original architecture. For instance, the authors of *BERT*, introduced in [24], proposed a language representation model that is pretrained on specially designed tasks to later boost its quality on the downstream task. Just like in the case of the original transformer architecture, the proposed BERT model outperformed other architectures in many classification tasks, especially in the area of Natural Language Processing. Following the success of the proposed approach, researchers have developed even better architectures. One of the recently developed models include *ALBERT*, proposed in [26], that is a lite version of the BERT model. The other interesting approach is taken in [27], which trains the BERT model adversarially. Besides it, several components of the baseline architecture have been improved over time, for instance the authors of [25] showed that changing the location of normalization layers lead to better performance of the model.

Motivated by the recent advancements in the transformer-based models, we decided to tackle to the problem of knowledge graph completion, using the above-mentioned models. In particular, we explore both context-free and contextualised methods, determining whether a transformer can benefit from an additional context information. Besides it, we compare the developed methods with the related models on two benchmark datasets, known as WN18RR and FB15K-237.

2. Background

In this chapter we will review the theory behind the techniques used to complete knowledge graphs. *Section* 2.1 is devoted to the basic properties and concepts of neural networks. In the subsequent sections we discuss more specialized models that are used to tackle the stated problem. In *Section* 2.2 and *Section* 2.3 we cover models learning graph representations. *Section* 2.4 provides an overview of how reinforcement learning can be utilized to complete knowledge graphs. In *Section* 2.5 we discuss the transformer architecture, which is the main building block for our methods. Finally, in *Section* 2.6 we show how the methods discussed in the previous sections have been utilized in the past to solve the considered problem.

2.1. Artificial neural networks

Neural networks are machine learning models inspired by a human brain. While the first neural models have been proposed decades ago, their popularity was very limited due to the poor performance. In the recent few years, the situation has changed as researchers developed sophisticated algorithms to optimize such models while in parallel computing resources have been grown significantly. At this point, neural networks have dominated other approaches to artificial intelligence, finding applications in practically every area of human life.

2.1.1. Feed-forward neural networks

Formally, a neural network is a complex mathematical function that maps input vectors to output vectors. One of the simplest neural network can be defined using the formula

$$y = f(Wx + b) \ , \tag{2.1}$$

where x, y denotes input and output vectors of size n, m respectively, W is a $n \times m$ matrix of parameters, b denotes a so-called bias vector of size m and f is a fixed activation function that adds non-linearity to our formula. The more complex neural network would repeat the process of mapping vectors several times e.g.

$$y = f_3(f_2(f_1(W_1x + b_1)W_2 + b_2)W_3 + b_3) \ . \tag{2.2}$$

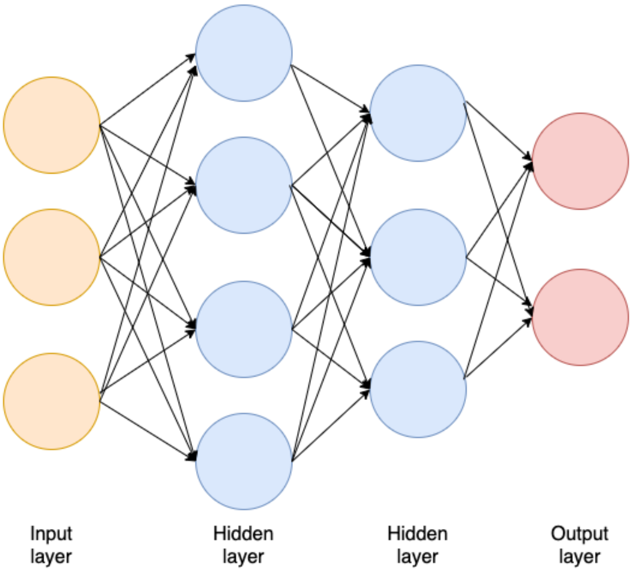


Figure 2.1: An example of a feed-forward network containing 2 hidden layers (marked in blue). The input layer (marked in orange) is composed of three neurons, while the output layer (marked in red) is composed of two neurons.

Due to its linear form, such network is often called a feed-forward neural network. An input vector x is often called an input layer, the intermediate vectors are called hidden layers and an output vector y is called an output later. The above-defined neural network has 2 hidden layers, defined as outputs of f_2 and f_3 activation functions. A feed-forward neural network can be illustrated in the form presented in *Figure* 2.1.

While we have shown how a neural network maps input vectors to output vectors, it is still unclear how such model can be leveraged to make predictions. The idea is to utilise so-called training dataset that is composed of input, expected output pairs. It is used to learn our neural network how to map inputs to outputs. In order to make use of the training dataset, one needs to convert given inputs and outputs to real-valued vectors. As neural networks are supervised on training data, they belong to the subcategory of machine learning called supervised learning. After training a neural network, its quality is rated on a validation dataset, which is disjoint with training dataset, providing an estimation of quality for examples that were not seen by the model. In particular, neural networks are known for fitting to training data too tightly while providing a poor quality on unseen examples. The techniques for preventing this phenomena, called overfitting, are discussed in *Subsection* 2.1.5. In case multiple models are tested, the validation set is used to pick the best one, while the quality of the chosen model is additionally evaluated on a test dataset as it can be a little biased to the validation dataset. The task-specific functions that rate models are often called evaluation metrics.

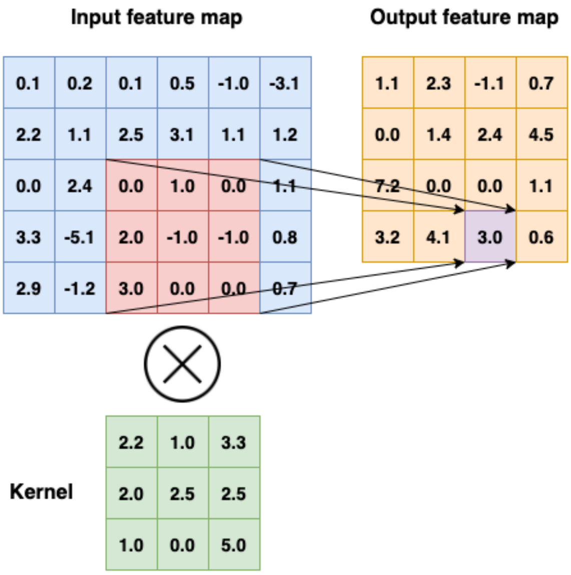
In order to fit a neural network to a given training dataset, one needs to find parameters that provide the best correspondence between predicted output vectors and expected output vectors. The trainable parameters include linear transformation matrices and bias vectors. For instance, for a neural network defined by *Equation* 2.2, the trainable parameters include $W_1, W_2, W_3, b_1, b_2, b_3$. Intuitively, the more parameters the network has, the higher its expressiveness. The optimization process of neural networks is performed by a specially designed algorithm that is described in *Subsection* 2.1.4.

2.1.2. Convolutional neural networks

Consider a task of classifying images into one of given categories e.g. $C = \{cat, dog\}$. It is easy to develop a feed-forward neural network that would treat images as input vectors and apply a few layers in order to obtain 1-dimensional output, representing a probability of an image to represent a cat. Actually, this approach works decently, but it suffers from the overfitting problem, causing that the quality of such model on unseen examples is lower than expected. The problem with the feed-forward approach is that such network tries to learn the dependencies between all pixels at the same time. The more natural way would be to train a model to firstly learn some low-level patterns like edges and then to recognize larger objects. Convolutional networks are models that implement this idea, enforcing the model to learn from neighbouring features.

In the case of convolutional networks, an input vector is represented by a 3-dimensional tensor of size $H \times W \times C$ interpreted as a height, width and the number of channels respectively. A single convolutional layer maps the input tensor, often called an input feature map, to the output tensor, which is called an output feature map. A single output neuron is computed by multiplying (element-wise) a patch of input feature map with a learnable 3D matrix of size $\tilde{h} \times \tilde{w} \times C$. The process is repeated by going through the input feature map with a sliding window of size $\tilde{h} \times \tilde{w} \times C$. The whole process for an input feature map with the number of channels $C = 1$ is shown in *Figure* 2.2. The above-defined algorithm maps an input feature map of size $H \times W \times C$ to an output feature map of size $\tilde{H} \times \tilde{W} \times 1$, using a learnable kernel matrix of size $\tilde{h} \times \tilde{w} \times C$. In practice, this process is repeated $\tilde{C}$ times for independent kernel matrices, where $\tilde{C}$ is called the number of filters. In this case, the output feature map is of size $\tilde{H} \times \tilde{W} \times \tilde{C}$.

Convolutional networks are learnt by modifying parameters contained in kernel matrices. Mathematically, nothing prevents composing a neural network that contains a few convolutional layers followed by feed-forward layers. In the first case inputs can be treated as 3D tensors, while in the latter case, they can be transformed to 1D representations.



Input feature map

0.1	0.2	0.1	0.5	-1.0	-3.1
2.2	1.1	2.5	3.1	1.1	1.2
0.0	2.4	0.0	1.0	0.0	1.1
3.3	-5.1	2.0	-1.0	-1.0	0.8
2.9	-1.2	3.0	0.0	0.0	0.7

Output feature map

1.1	2.3	-1.1	0.7
0.0	1.4	2.4	4.5
7.2	0.0	0.0	1.1
3.2	4.1	3.0	0.6

Kernel

2.2	1.0	3.3
2.0	2.5	2.5
1.0	0.0	5.0

Figure 2.2: An example of how convolutional layer maps input feature map (marked in blue) to output feature map (marked in orange). A single patch (marked in red) is multiplied element-wise with a learnable kernel matrix (marked in green) in order to produce one output feature (marked in purple). A sliding window goes though the entire image, multiplying input patches with a kernel matrix. Note that while in this example an input feature map contains only one channel, in the more general case of C channels, the kernel matrix would be of size $C \times 3 \times 3$.

2.1.3. Loss functions

In order to train a model, one needs to define a similarity between predicted outputs $\tilde{y}$ and ground-truth outputs y. A function that defines this similarity is called a loss function and depends on a considered task. One popular case is when a target variable y is continuous and the loss function should be based on the distance between y and $\tilde{y}$. In the field of machine learning, this is often called a regression task. While many different functions can be designed to optimize such model, the most popular one is

$$L_2(y, \tilde{y}) = ||y - \tilde{y}||_2 = \sum_i (y_i - \tilde{y}_i)^2 \ ,$$

which is called L2 loss function. The other case is when $\tilde{y}$ represents an unnormalised probability distribution for a set of established classes (e.g. $C = \{cat, dog, rabbit\}$), while y is so-called one-hot vector encoding classes that are true for a specific sample as 1.0 and classes that are false as 0.0. In this case, the popular choice is to first apply a softmax function to normalize $\tilde{y}$

$$\hat{y}_i = \frac{e^{\tilde{y}_i}}{\sum_j e^{\tilde{y}_j}}$$

and then apply cross-entropy loss function

$$L(y, \hat{y}) = -\sum_i y_i log(\hat{y}_i) \ ,$$

penalizing predictions for classes for which $y_i > 0$. Except natural intuitions that the above-defined loss function should be minimized in order to provide a good estimate of y, it has also mathematical foundations that can be found in [10]. In case there are only two classes, the discussed loss function is often called binary cross entropy, while the task of optimising such function is referred as binary classification.

2.1.4. Optimization

In the previous subsections we mentioned that a neural network is optimized by adjusting parameters contained in matrices and bias vectors. Besides it, we defined a loss function that should be minimised in order to fit to the expected outputs. In this subsection, we show how to actually minimize a loss function.

First of all, our training data samples should be split into batches of fixed size B, which is often referred as batch size. In each training step, a batch of inputs is pushed to a model, and its parameters are slightly modified to lower the value of a loss function. In order to minimize it, a technique called gradient descent is utilised. Specifically, it computes a gradient of the loss function with respect to all parameters, using so-called backpropagation algorithm. As a result, the method obtains a vector that defines the direction that should be followed to lower the value of the loss function. Then, the vector of parameters is updated by applying

$$\theta_{k+1} = \theta_k - \alpha \nabla_\theta L(\tilde{Y}, Y) \ ,$$

where α is called a learning rate. The process of updating parameters is performed for all training batches and repeated E times, where E is referred as the number of epochs. While this naive algorithm can stuck in a local minima, several advancements have been developed in order to make it possible to converge to a global minima. One of the currently popular approach is known as Adam optimizer, introduced in [7]. Over time, researchers have also developed specialized layers that increase the convergence rate. One of the most successful layers is Batch Normalization, proposed in [6], normalizing batches of inputs to the parameterised Gaussian distribution. The other popular alternative is Layer Normalization, introduced in [9], which normalizes each sample separately, making the computations more precise for small batch sizes.

2.1.5. Preventing overfitting

Neural networks are great in recognising patterns in training data. In particular, a feed-forward neural network with 1 hidden layer can represent any function. But in practice, we are not interested in a model that remembers all training data samples i.e. overfits to them. Instead, we would like to design models that generalize well, providing good quality of predictions on unseen examples.

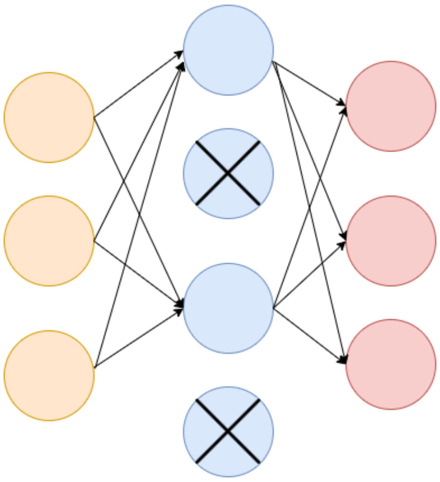


Figure 2.3: An illustration of dropout to applied to a hidden layer (marked in blue). The crossed out neurons are set to 0.0, which has an effect of ignoring their input and output connections. In this case dropout rate $r = 0.5$.

One popular way of enforcing the network to generalize is adding a dropout layer [4]. The idea is to (in each training step) set some random subset of neurons after a specific layer to 0.0 and rescale the other neurons by 1.0 / $(1.0 - r)$, where r (often called a dropout rate) denotes the percentage of neurons that are set to 0.0. The neurons that are set to 0.0 can be treated as removed. The intuitive explanation of how dropout is applied during the training process, is shown in *Figure* 2.3. During the evaluation of the network on unseen examples, all neurons are included and no rescaling is applied. The intuition behind this approach is that it enforces the network to spread out its weights to many neurons rather than relying on a small number of connections.

The other technique to reduce the overfitting is to add an additional loss that penalizes model's parameters. The common way of applying this idea is to add a regularization term to the loss function

$$L(y, \tilde{y})^{\theta} = L_m^{\theta}(y, \tilde{y}) + \lambda \sum_i \theta_i^2 \ ,$$

where θ denotes a vector of parameters, L_m is the loss given by the model and λ is a parameter controlling the regularization strength. The above-defined technique is often called a weight decay. The intuition behind this approach is that it enforces the network to keep parameter values close to 0.0 and to avoid extreme values, making it less flexible.

The other regularization technique, which is designed for classification tasks, is label smoothing. The idea behind this method is to replace hard $c \in \{0, 1\}$ labels with their soft versions. Specifically, when label smoothing parameter is set to $s \in (0, 1)$, true labels are replaced with $(1 - s) + s \;/\; N$, while false labels are replaced with $s \;/\; N$, where N denotes the total number of classes. The main motivation behind this approach is that the training dataset can contain mistakenly labeled examples. Another common situation is when multiple output labels are correct, while a dataset is constructed in a way that only one label is true for a specific sample. In this case, label smoothing encourages a model to assign some non-zero probability to each class. In particular, it can assign higher probabilities to labels that may be correct.

2.2. Graph embedding methods

Consider a dataset containing users' features and the problem of classifying each user to one the specified categories. In order to tackle this task, one may utilise neural networks discussed in *Section* 2.1 to learn a mapping from user's features to categories. Now, let's assume that one of our features is a list of friends of a user. In other words, users are interconnected, forming a graph. While we could try to naively encode this information by creating a one-hot vector indicating a list of friends for each user, there are more sophisticated ways to include this information. One of the most successful approaches is to use graph embedding methods that aim to learn low-dimensional vector representations of nodes.

2.2.1. Classification of graph embedding methods

Most of embedding methods are unsupervised. The goal is to produce generic, continuous representations of nodes based on their connectivity. The representation of a node is often referred as embedding. The learnt embeddings can be later used by some supervised model to perform a node classification task (e.g. classify users of a social network), link prediction task (e.g. predict new friendships) or graph classification task (e.g. classifying chemical structures). Most of embedding methods are based on so-called homophily hypothesis, which says that nodes that are highly interconnected and belong to similar network clusters should have similar embeddings. The other category of considered methods is based on structural equivalence hypothesis, which states that nodes with similar structural roles in a graph should be embedded closely together. Lastly, while most of methods allow to learn only fixed representations for nodes contained in the training dataset i.e. transductive methods, there exist more specialized methods allowing predictions to be made on unseen nodes i.e. inductive methods.

2.2.2. DeepWalk algorithm and its extensions

One of the baseline models that outclassed previous approaches is DeepWalk, introduced in [5]. At each step of the algorithm, a random node $v \in V$ is chosen. Then, a random path $W = \{w_1, w_2, \ldots, w_k\}$ is constructed by starting in the node v and repeatedly going to one of the neighbours of the last node on the constructed path. The generated paths are later used to enforce nodes having similar neighbours to be closely embedded. Specifically, let $v_j \in W$ be a random node from the generated path and its context to be defined as a set of nodes $K = \{w_{j-c}, w_{j-c+1}, \ldots, w_{j+1}, w_{j+c}\}$. Now, draw one vertex $v_c \in K$ and define $p(v_c|v_j)$ with the formula

$$p(v_c|v_j) = \frac{e^{R_j C_c^T}}{\sum_k e^{R_j C_k^T}} \ , \tag{2.3}$$

where R_i denotes the i-th row of the learnable embeddings matrix, while C_i is the i-th row of the learnable context matrix. The goal of the above-defined model is to maximize this probability for the generated v_j, v_c nodes. As a byproduct of this procedure, we get the embeddings matrix R, such that the i-th row represents the i-th node. The intuition behind this approach is it enforces nodes that have many common neighbours to have similar embeddings as they are often multiplied with the same context vectors. A toy example of how the presented algorithm could embed a small graph in 2-dimensional space is shown in *Figure* 2.4.

Interestingly, the presented algorithm was invented previously to embed words in a way that the related ones have similar representations. The original method is called the Skip-gram model and was introduced in [2]. Additionally, to speed up the computation time of *Equation* 2.3, the authors proposed to replace the original softmax function with a hierarchical softmax, keeping nodes in leaves of a binary tree. The other popular method is to use negative sampling, which tries to maximize

$$p(v_c|v_j) = e^{R_j C_c^T}$$

for positive pairs, while minimizing the same formula for negative pairs that are created by drawing two random words. The analogous extensions can be applied to the DeepWalk algorithm.

While the original DeepWalk algorithm traverses the graph using DFS strategy, other strategies could be utilised. The authors of [11] generalized DeepWalk to choose between one of strategies: BFS, DFS, going back to the previous node. The proposed node2vec algorithm interleaves strategies by selecting a random one in each step of constructing the path. A distribution defining the probability of choosing a specific strategy impacts the learnt representations. Most commonly, the parameters defining a distribution of strategies are finetuned to provide the best quality.

The other interesting extension proposed in [14] utilises the DeepWalk algorithm to embed nodes that have similar structural roles closely together. The idea behind struc2vec is to first construct a graph encoding structural similarities between nodes and then learn embeddings by performing random walks. The authors proposed to define a structural distance between nodes $u, v \in V$ based on the number of

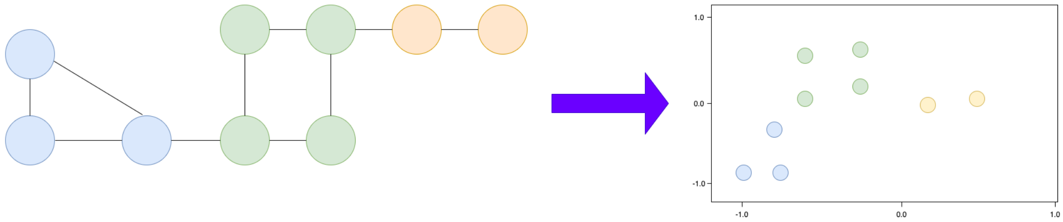


Figure 2.4: An example of how DeepWalk algorithm could embed nodes of a given graph in 2 dimensional space. The nodes are marked with colors to show the correspondence between the locations in the graph and locations in the embedding space.

neighbours $R_k(u), R_k(v)$ at specified distances $k \in \{1, \ldots, K\}$. Then, the constructed distances matrix is utilized to define the probability of transitioning from u to v. As a result, random walks enforce nodes of the same structure to have similar embeddings.

2.2.3. Learning representations of unseen nodes

Though we have shown many extensions of the DeepWalk algorithm, none of them scale to unseen nodes. The naive approach to extend it would be to rerun random walks when new nodes arrive, but it makes the computations very costly. In case the nodes are represented by additional pre-defined features, one may try to learn embeddings by mapping input features. One way of applying this idea is to use a model introduced in [12]. The authors propose to learn a specific supervised task along with the embeddings of nodes at the same time. Specifically, one of hidden layers of the supervised model can be treated as an embedding layer, representing an input node with a given features. In order to enforce the neighbouring nodes to have similar embeddings, random walks are applied to the embedding layer, causing the information about the neighbourhood to backpropagate to the input layer. The model is trained jointly on the supervised task and random walks.

The other popular approach, introduced in [13], learns embeddings without a use of additional features. The idea of the authors is to apply a few feed-forward layers to map an adjacency vector of a specific node to its embedding e_n and then apply a few more feed-forward layers in order to reconstruct the input adjacency vector. Except the reconstruction loss between the original adjacency vector and the reconstructed vector, additional L2 loss is applied between embeddings e_n of neighbouring nodes, enforcing them to lie close to each other. The model is trained on both tasks jointly, ensuring that embeddings have the two above-defined properties.

2.3. Graph neural networks

In *Section* 2.2 we have shown how to learn generic representations of nodes, encoding the information about the neighbourhood. In the present section, we will show how to learn task-specific embeddings. Firstly, we will define the notion of message passing, showing how it can be leveraged to exchange the information between nodes. Then, we will present a few approaches that utilise this technique to boost predictions quality of supervised models.

2.3.1. Message passing

Passing messages between processes is a very known technique in computer science. In the context of this thesis, we will consider a graph, whose neighbouring nodes exchange some information by sending and receiving messages. Formally, assume that each node i has been assigned some representation $h_i^{(0)}$. In the k-th step, we will assign the (k + 1)-th representation of the node i by applying

$$h_i^{(k+1)} = f_k(h_i^{(k)}, \{h_j^{(k)} : j \in N(i)\}) \ , \tag{2.4}$$

where $N(i)$ denotes the neighbours of the node i and f_k is an aggregation function. An example illustrating the described procedure is shown in *Figure* 2.5. This process is performed for each node and repeated K times, allowing a node to obtain messages from its k-hop neighbourhood. The final representations $h_i^{(K)}$ are utilised to perform the desired classification or regression task. In order to perform the backpropagation and update parameters of aggregation functions f_k, they must be differentiable.

Interestingly, all graph neural networks models can be formulated with *Equation* 2.4. The main difference between the models is the definition of the aggregation functions f_k. The other difference is how the final representations $h_i^{(K)}$ are used. In the simplest case, one may perform a node classification task. On the other side, the final representations can be aggregated to perform a link prediction or even a graph classification task. Additionally, the above-defined message passing formulation can be easily extended to take into account different edge types or features.

In case initial representations $h_i^{(0)}$ are fixed, new nodes can be added to a graph and used for the underlying classification or regression task, without much loss of quality. In the other case, one needs to start with a random representation of the added node and retrain the model to learn its representation. The other possibility is to use graph embedding methods discussed in *Section* 2.2.

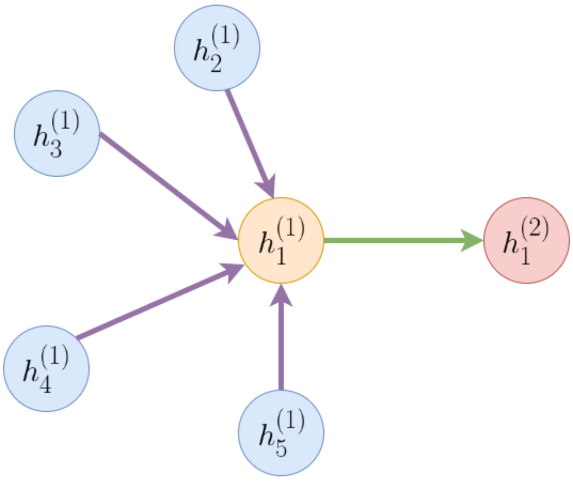


Figure 2.5: An example of how message passing is used to exchange the information between nodes. The embedding $h_1^{(1)}$ (marked in orange) of the node h_1 is updated by aggregating the embeddings of its neighbours (marked in blue). This process results in the new embedding $h_1^{(2)}$ of the node h_1 (marked in red).

2.3.2. Overview of models

Over time, researchers have developed multiple ways of modelling aggregating functions f_k. One of the most successful approaches, proposed in [23], utilises the following aggregation function

$$H^{(k+1)} = f_k(H^{(k)}) = \sigma(\tilde{D}^{-\frac{1}{2}}\tilde{A}\tilde{D}^{-\frac{1}{2}}H^{(k)}W^{(k)})) \ ,$$

where σ denotes an activation function, $\tilde{A}$ is the adjacency matrix with added self-loops, D is a diagonal matrix, such that D_{ii} represents the order of the node i and W is layer-specific trainable matrix. The formula has its mathematical justification, relying on the graph Laplacian. From the more intuitive point of view, $\tilde{D}^{-\frac{1}{2}}\tilde{A}\tilde{D}^{-\frac{1}{2}}$ can be thought of a convolution matrix that is based on the connectivity of nodes. The discussed model is called GCN and has been successfully applied to many tasks involving graphs.

The other popular choice for the aggregation functions f_k, proposed in [16], is Long Short-Term Memory (LSTM). In short, LSTM is a recurrent model that can take variable-length inputs, in parallel reducing the well-known vanishing gradient problem. More details of the LSTM model can be found in [10].

Yet another approach is to use a so-called self-attention mechanism that is discussed more deeply in *Subsection* 2.5.1. In the context of graph neural networks, the above-mentioned mechanism is used to learn how much attention should be put to a specific neighbour, when receiving its message. Specifically, let $\alpha_{ij} \in [0, 1]$ be a learnable weight, denoting how much attention the node i should put to its neighbour node j

and for non-neighbouring nodes set $\alpha_{ij} = 0.0$. Now, let the aggregation function be defined by the following formula

$$h_i^{(k+1)} = f_k(h_i^{(k)}, K) = \sigma(\sum_{h_j^{(k)} \in K} \alpha_{ij}^{(k)} W^{(k)} h_j^{(k)}) \ ,$$

where K denotes the i-th node neighbours, σ is an activation function and $W^{(k)}$ is a learnable matrix. Additionally, in order to take into account the current representation of the node i, self-connections are added to the graph. The model is optimized to update attention weights α and parameter matrices $W^{(k)}$, providing additional insights on the importance of specific neighbours.

2.4. Reinforcement learning

Consider a supervised model whose goal is to learn to play a computer game. It makes some decisions and based on them, the environment provides it new states. In this situation, the model does not know whether it made the right decision. As a result, it is not provided the ground-truth labels and cannot be supervised. This type of problem, which involves maximizing the long-time reward based on a sequence of decisions, concerns the area of machine learning called Reinforcement learning. Formally, the goal of this learning method is to find a function π that maximizes the so-called utility function

$$U^{\pi}(s) = \mathbb{E}(\sum_{t=0}^{\infty} \gamma^t R(s_t) | \pi, s = s_0) \ ,$$

where π is a policy function that defines the actions taken by the model, s_t denotes the t-th state of the game, $R(s_t)$ is a function that assigns a reward to a given state and $\gamma \in (0, 1)$ is a constant lowering the rewards that are given in the later stage of the game. While the policy π is deterministic, the environment can be nondeterministic (e.g. the provided state can be based not only on our actions, but also on how the other player reacts), thus the expected value is applied. The naive way of finding the optimal policy would be to observe that the optimal utility function is defined by

$$U^{\star}(s) = R(s) + \gamma max_a \sum_{s'} P(s, a, s') U(s')$$

for each $s \in S$, where $P(s, a, s')$ denotes the probability of landing in the state s', assuming that the current state is s and that the action a was taken. These equations are called the Bellman equations and while they are not linear, there exist an iterative algorithm for solving the system of such equations.

In practise, the state space is too large to directly solve the system of Bellman equations. The common solution is to use a function approximating utility function

U. It can be any learnable model and in particular, the most common choice is to use a neural network. In order to learn the approximation function U, one may supervise it by simulating some decisions. Instead of performing the exact simulation, it is common to rely on some approximations that are obtained using Monte Carlo methods. These ideas lead to popular Reinforcement learning algorithms, called Q-learning and Policy Gradients. More details behind the presented methods can be found in [8].

2.5. Transformers

Before the rise of transformers, sequence-to-sequence tasks were modelled with recurrent neural networks. These approaches have had many problems as vanishing gradients, causing the quality of models to degrade for long sequences of inputs. While researches have developed many approaches to reduce this issue, training recurrent models was still inefficient due to their inability to being parallelized. Indeed, the main assumption behind recurrent neural networks is that the outputs of the k-th step cannot be inferred until the outputs of all previous $k - 1$ steps have been calculated. The situation has changed when researchers have proposed [17], introducing the transformer architecture that get rid of all the above-mentioned issues. In the following subsections we define the key components of the proposed transformer architecture and the extensions that have been developed over time.

2.5.1. Self-attention mechanism

In the abstract form, attention mechanism can be defined as mapping a given query Q and a list of n key-value pairs (K, V) to output values. More formally, we assume that a query Q is a matrix of size $1 \times d_k$, while a list of keys and their corresponding values form the matrices K and V of size $n \times d_k$. While the attention mechanism can be modelled in many ways, one of the most popular forms is the so-called scaled dot-product attention

$$attention(Q, K, V) = softmax(\frac{QK^T}{\sqrt{d_k}})V \ , \tag{2.5}$$

where d_k is used to scale the computed weights. The illustration of the above-defined mechanism is shown in *Figure* 2.6. Intuitively, it computes a convex sum of values, based on the similarity of the corresponding keys with the query Q. When $Q = K = V$, the described mechanism is called self-attention. Additionally, one may define attention weights, which in case of the self-attention have the form

$$\alpha_{ij} = softmax(\frac{QK^T}{\sqrt{d_k}})_{ij} = softmax(\frac{VV^T}{\sqrt{d_k}})_{ij} \ ,$$

which indicate how much attention the i-th value (query) puts to the j-th value. Indeed, the attention mechanism was developed in order to learn how much attention

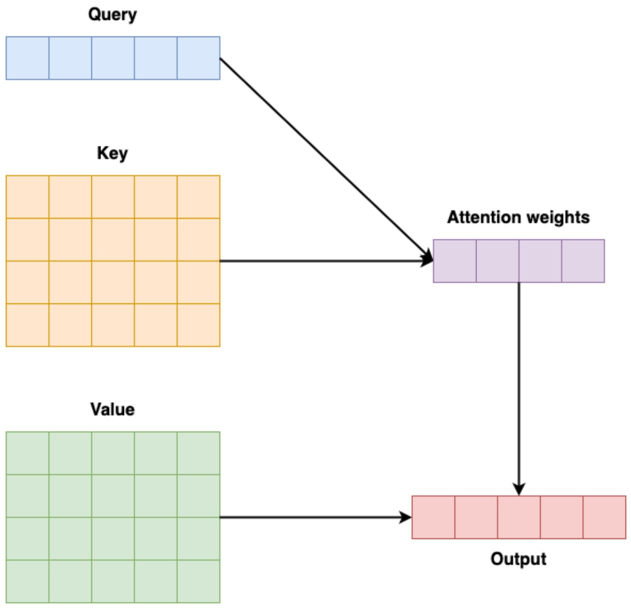


Figure 2.6: An illustration of the attention mechanism. In the first stage of the procedure, a query (marked in blue) and keys (marked in orange) are used to compute attention weights (marked in purple). Then, the output (marked in red) is formed by multiplying a matrix of attention weights with a matrix of values i.e. a convex combination of values is computed.

should be put into other elements of a sequence. Over time, several extensions of the *Equation* 2.5 have been proposed to enable the model to learn better-suited combinations of values V e.g.

$$attention(Q, K, V) = softmax(\frac{(QW_Q)(KW_K)^T}{\sqrt{d_k}})(VW_V) \ ,$$

where W_K, W_V, W_Q are learnable matrices mapping keys, values and query, enabling the dot-product between the query and keys to be computed in the custom space as well as allowing values to be linearly transformed.

The introduced self-attention mechanism is the key component of the transformer layer that will be discussed more deeply in *Subsection* 2.5.4. In particular, it makes use of multiple attention mechanisms, each learnt using an independent linear transformations of input keys, values and queries. The outputs of all attention mechanisms are concatenated and projected the final output, using learnable matrix. This mechanism is called Multi-Head Attention and is often used instead of a single attention function. Intuitively, this extension allows the model to spread its attention to different features by adjusting attention weights of each attention head.

2.5.2. Pointwise feed-forward layer

While the attention mechanism allows a model to exchange the information between elements of a sequence, the elements may need to update their representations by itself. One of the most intuitive ways to model it, would be to use a few feed-forward layers, introduced in *Subsection* 2.1.1, for each element of the sequence independently. The layer that follows this pattern is called the pointwise feed-forward layer. Formally, it takes a matrix of elements of a sequence and applies a few linear transformations, each followed by an activation function. Importantly, the same transformations are applied to all elements of the sequence. This means that a model is enforced to learn generic transformations, regardless of the characteristics of a specific element.

2.5.3. Positional embeddings

It's a common case that the order of input sequence elements is important. For instance, consider a task of translating a sentence from one language to another. In this task, different permutations of words can lead to various semantics of the whole sentence. In order to encode the information about positions of the elements, one may keep a vector representation of each position and then merge it with a representation of an element on a specific position. Such representation of a position is often referred as a positional embedding.

The representation of an element can be merged with a position embedding by concatenating their vectors. In case both vectors have the same dimensionality, instead of concatenation, it is common to sum the corresponding embeddings element-wise. One approach to assign a representation to a word is to come up with a function that could identify each position uniquely. In this case, the most popular choice is to use the one based on different frequencies of some cyclic functions e.g.

$$PE_{(p,k)} = \begin{cases} sin(\frac{p}{100000^{k/d}}) & \text{if } k = 2i \\ cos(\frac{p}{100000^{k/d}}) & \text{if } k = 2i+1 \end{cases},$$

where p is a position that will be represented by an embedding, i refers to an individual dimension of the embedding and d denotes the total number of dimensions. The other popular choice is to start with random positional embeddings and update them during the training process, based on the gradient information.

2.5.4. Transformer encoder and decoder

The introduced multi-head self-attention layer along with the pointwise feed-forward layer form together a transformer layer, which is illustrated in *Figure* 2.7. The idea behind this layer is to exchange the information between the elements of a sequence and then update each element independently, leveraging the two above-mentioned sublayers. Additionally, in order to increase the flow of information, skip connections between the sublayers are applied. Specifically, the outputs of the attention sublayer are summed with the original inputs as well as the outputs of the pointwise sublayer are summed with the outputs of the attention layer. This allows the model to utilise the information contained in the previous layers. Besides, it reduces the vanishing gradients problem i.e when the gradient is vanishingly small.

The transformer encoder is composed of a few stacked transformer layers. It takes a sequence of n input elements, represented by their embeddings (with optionally positional embeddings applied), and returns a sequence of n embeddings, each representing the corresponding input element in the context of other elements. Similarly to the encoder, the decoder is composed of a few transformer layers. The main distinction is that it takes a sequence of n output elements along with the outputs of the encoder. Most commonly, the outputs of the encoder are injected after a few first transformer layers by summing the output vectors element-wise. The sequence of output elements is often used to provide an information about the previous outputs. For instance, in the machine translation task, it's common to translate a sentence word by word. In this case, the output sequence could contain a partial translation of the input sequence.

The outputs of the decoder are used to supervise a model. The computed gradients are backpropagated back to the inputs of the encoder, allowing the decoder and encoder to be updated simultaneously. In case some input elements should not be visible by other elements, the corresponding attention weights are set to 0.0. The introduced layers and techniques form together the original transformer architecture, introduced in [17]. The model was developed with natural language processing applications in mind, but can be used in any sequence-to-sequence tasks.

2.5.5. Extensions to the original transformer architecture

Over time, several extensions to the original model were proposed. One of the most successful ones include BERT, introduced in [24]. In contrast to the original transformer architecture, it works only an input sequence. This makes it better suited for the tasks, in which the whole output sequence is expected to be predicted in one pass. As a result, the BERT model utilizes only the encoder part of the original transformer model. Additionally, the authors proposed to pretrain the proposed model on two tasks: restoring the masked input word and predicting the next sentence. The proposed approach effectively reduces the training time on the downstream task, leveraging the knowledge obtained during the pretraining process. Furthermore, the model was later extended in [26] to share the parameters of transformer layers, making it more parameter-efficient.

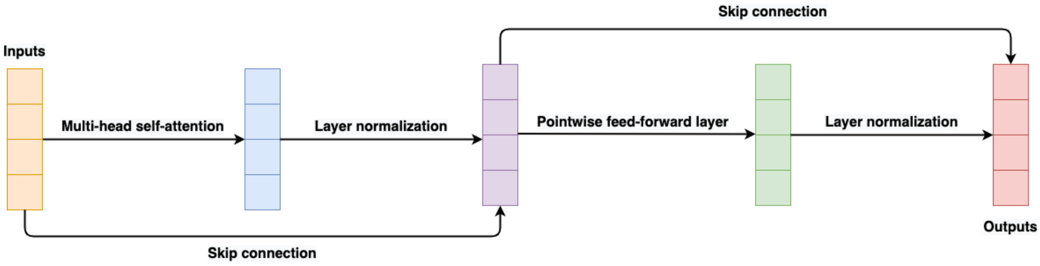


Figure 2.7: An illustration of the transformer layer. Given an input sequence with the encoded positions (marked in orange), the layer first applies the self-attention mechanism to allow the elements to exchange the information. Then, the outputs of the attention layer (marked in blue) are normalized and merged with the original inputs (marked in purple). Afterwards, each element of the sequence is transformed independently with the pointwise feed-forward layer (marked in green). Finally, the elements are normalized and merged with the outputs of the attention layer, forming the output embeddings (marked in red).

Another recently developed extension of the transformer architecture is ELECTRA, introduced in [27]. The authors proposed to train two models in parallel, called generator and discriminator. The generator takes as its input a sequence of elements, with roughly 15% of random tokens masked out. Its goal is to predict the masked tokens, using a few transformer layers followed by softmax. Then, the output distribution is utilised to sample a token for each position, forming a sequence s_G. The constructed sequence s_G is then pushed as an input of the discriminator, which is trained to recognise which tokens are real, considering the remaining ones as fake.

At first, the presented ELECTRA model may seem indistinguishable from Generative Adversarial Networks (GANs), introduced in [3]. However, if one delves into the details, there are several differences. Firstly, in the case ELECTRA, the gradients of the generator and the discriminator are disjoint, causing the information not to flow from one model the other one one. The other distinction is that the generator is trained to generate real samples that are leveraged by the discriminator, unlike in GANs where the discriminator tries to generate fake samples that are pushed as inputs to the generator. Lastly, after the training procedure is finished, ELECTRA throws out the generator instead of the discriminator. In particular, the whole procedure can be treated as the form of pretraining as the discriminator is further used to train the model on the downstream task.

2.6. Models proposed for the graph completion problem

In this section, we will present the related work on the knowledge graph completion problem. The methods will be presented from the simplest context-free ones that are based on convolutional networks to the more advanced contextualised ones based on reinforcement learning or graph neural networks. While in the recent few years hundreds of different methods have been developed, we chose the ones that provided a significant quality boost compared to their predecessors. In parallel, we omit the methods that report inflated quality results due to improper evaluation protocol.

2.6.1. Context-free methods

One of the most influential idea to tackle the problem of knowledge graph completion, was to represent entities and relations by low-dimensional continuous vectors, called embeddings. The most known model applying this idea is **TransE**, introduced in [1]. The authors proposed to start with random embeddings of entities and relations, then iteratively update them by optimizing the model with the following loss function

$$L(h,r,t,h',t') = max(0, ||h+r-t||_2 - ||h'+r-t'||_2 + \gamma) \ ,$$

where (h,r,t) represents a (positive) triple that belongs to the knowledge graph, while a (negative) triple (h',r,t') is formed by replacing either h or t, with a random entity. Intuitively, this model tries to rotate vectors representing entities and relations in a way that the norm of the expression $||h+r-t||_2$ is higher for positive triples than for negative triples. Additionally, the margin parameter γ controls how high the difference between the norms should be in order to have 0.0 loss. Interestingly, the discussed architecture can be treated as a 1D convolution layer of $D \times 3$ image with fixed $(1,1,-1)$ kernel. The TransE model was further extended to **STransE** in [15] to allow relation-specific embeddings of entities. More formally, the authors replaced the expression $||h+r-t||_2$ with $||W_{h,r}h+r-W_{t,r}t||_2$, allowing more flexible representations.

In the recent years, many improvements to the TransE model have been proposed. In particular, several methods applying convolutional layers on top of embeddings have been developed. For instance, in [19] the authors proposed **ConvE** model that concatenates the known head/tail entity embedding with the relation embedding, forming $D \times 2$ image. After that, a convolutional layer, followed by a feed-forward projection layer, are applied to obtain the output embedding e_o of dimensionality D. Finally, a dot-product between e_o and each entity $e \in E$ is computed to find the most similar entity to e_o. The model is supervised by a softmax function that is used to maximize the similarity between e_o and the-ground truth tail/head entity that should be predicted. In order to allow the model to distinguish between input and output relations, separate relation embeddings are used for head and tail entities. The model not only optimizes the weights of intermediate layers, but also finetunes entity and relation embeddings. Additionally, it makes use of Dropout and Label Smoothing to prevent overfitting.

2.6.2. Context-based methods

With the rise of machine learning models operating on graphs, several context-based methods for knowledge graph completion have been proposed. For instance, in [22] the authors introduced the **SACN** model, leveraging custom WGCN layer

$$h_i^{(k+1)} = \sigma(\sum_{j \in N(i)} \alpha_{r(i,j)} g(h_i^{(k)}, h_j^{(k)})) \ ,$$

where g specifies how to incorporate neighboring information and $r(i,j)$ denotes the relation that connects the i-th node with the j-th node. Intuitively, the idea is to make it possible for each relation to focus on different parts of the neighbouring embeddings. The proposed model is composed of a few WGCN layers that collect the information from the neighbourhood, forming the embedding of the source entity e_s. Then, a convolutional network is applied on top of the aggregated embedding e_s and input relation embedding, with the goal to predict the target entity. In particular, this architecture is similar to the ConvE model, except the fact that the embedding of the source entity is formed by aggregating neighbouring embeddings.

The downside of the model discussed above is that the representations of relations are not updated by the graph neural network itself. In particular, the only way the aggregation function can leverage relation-specific information is by adjusting attention weights. The other approach is presented in the **CompGCN** model, introduced in [29], where the representations of relations are used directly by the graph neural network. More precisely, the authors defined the aggregation function

$$h_i^{(k+1)} = \sigma(\sum_{j \in N(i)} W_{\lambda(r)} g(h_j^{(k)}, r_j^{(k)})) \ ,$$

where $r_j^{(k)}$ denotes the representation of the j-th relation in the context of the k-th aggregation function and $\lambda(r)$ is used to select one of three matrices, depending on the type of relation r. Specifically, the matrix $W_O^{(k)}$ is used for relations originally contained in the knowledge graph, $W_I^{(k)}$ is used for added inverse relations and $W_S^{(k)}$ is used for self-loops. This allows the information to flow in both sides, while keeping the number of model's parameters low. Additionally, the relation embeddings are transformed after each layer

$$r_i^{(k+1)} = \tilde{W} r_i^{(k)} \ ,$$

which makes the aggregation functions more flexible. Finally, the authors tested the proposed CompGCN model with multiple scoring functions applied on top of aggregated embeddings, including TransE and ConvE.

The other interesting approach was taken in [21], introducing the **MINERVA** model. The authors proposed to learn it to walk though a graph in order to find a missing head or tail entity. More specifically, given a source entity and a relation, the goal is to take a sequence of decisions that will lead to the target entity, where in each step the model can go to one of its neighbours or remain in the current node. After a fixed number of steps, in case the model lands in the target entity, it is given a reward. Additionally, in order to increase the awareness about the visited nodes, the history is included in the model's state.

3. Developed methods

In the following sections we will discuss our transformer-based approach in depth. We will start by introducing the main components, forming our context-free architecture. Then, we will go through the developed extensions, which add graph context to our model. Lastly, we will define the models that were selected for further experiments discussed in *Chapter* 4.

3.1. Context-free transformer architecture

Our model assigns latent representations (embeddings) to each entity and relation of a given knowledge graph. Additionally, we leverage positional embeddings discussed in 2.5.3 and model-specific embeddings of special tokens. We refer to the above-mentioned objects as tokens. In particular, we keep all tokens in one large vocabulary V and their embeddings in a matrix T of size $|V| \times D$, where D denotes the dimensionality of one token. The embedding of a token can be thought of its learnable representation. The details on how we initialize and train token embeddings are included *Subsection* 3.1.1.

The developed architecture takes as its input a batch samples, where each sample is composed of a sequence of input tokens. In case of context-free model, all input sequences are of length 3, while in other models different training batches may contain sequences of different lengths. Nevertheless, all input sequences of a specific training batch are expected to be of the same length. Each token is transformed to the corresponding embedding and then several transformer layers, introduced in *Subsection* 2.5.4, are applied to form the output sequence. This process can be interpreted as exchanging information between tokens, where each token can extract information from all other tokens and in particular, it can choose which information is useful using self-attention mechanism. The output sequence of contextualised tokens is used to supervise the model. The high-level overview of our model is shown in *Figure* 3.1. The details of sequence-to-sequence mapping component as well as loss functions are discussed more deeply in *Subsection* 3.1.2 and *Subsection* 3.1.3 respectively. Besides it, we highlight the importance of normalization layers in *Subsection* 3.1.4.

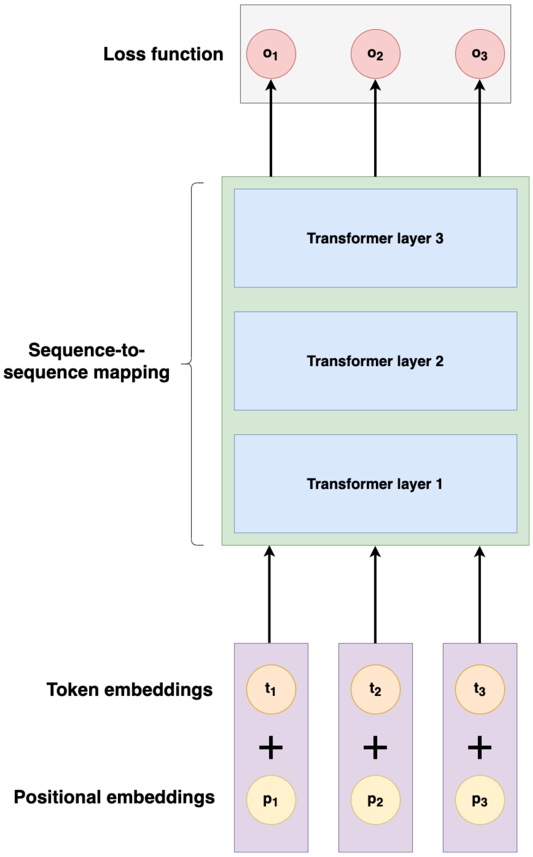


Figure 3.1: A high-level overview of our architecture. First, input tokens are mapped to their corresponding embeddings (marked in orange) and summed element-wise with positional embeddings (marked in yellow). The formed embeddings are marked in purple. Then, a few transformer layers (marked in blue), forming together sequence-to-sequence component (marked in green), are applied to map input sequence to output tokens. The outputs of the last layer (marked in red) are then passed to the loss function component (marked in gray) that supervise the whole model.

In case of context-free architecture, input tokens are partially masked triplets, representing edges contained in the training dataset. More specifically, for a given training triple (h, r, t), we mask out either head entity h or tail entity t. This forms either $([mask], r, t)$ or $(h, r, [mask])$ sequence, where $[mask]$ is a special token with a learnable embedding. In particular, for each edge we form both sequences and randomly shuffle all formed samples. After transforming tokens to their corresponding embeddings and applying sequence-to-sequence component, (h_c, r_c, t_c) sequence of embeddings is obtained. We interpret each embedding as a contextualised representation of the corresponding input token. Particularly, the model is supervised in a way that the output token on a position matching $[mask]$ input token is close to the h_e embedding/h_t embedding of the masked head/tail entity. The closer both embeddings are, the better the model is. Both variants of the masked head and tail entity are presented in *Figure* 3.2.

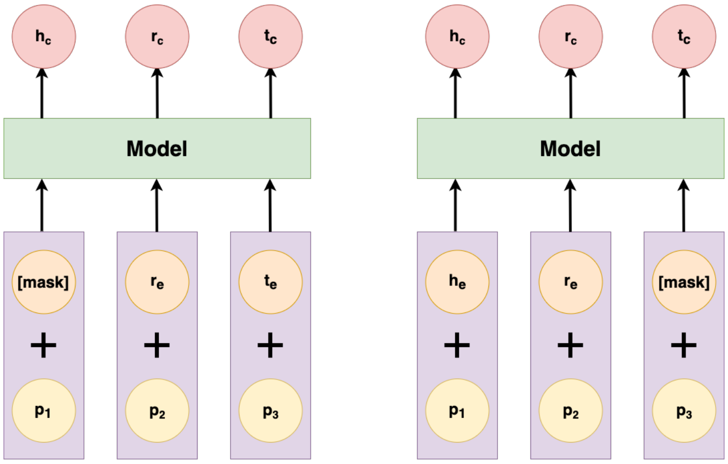


Figure 3.2: An illustration of input and output sequences of the developed context-free model. In the first case (on the left), head entity is masked out, while relation and tail entity embeddings are pushed to the model. The model is expected to restore the masked head entity. In the other case (on the right), tail entity is masked out and the model is learnt to restore it, given embeddings of relation and head entity.

3.1.1. Initialising and training token embeddings

We have explored various approaches for embeddings initialization. We found that initialising embeddings of all tokens with random values provides the best results. Importantly, the initialized values should in a small range $[-0.05, 0.05]$, otherwise the network loses its capability to learn anything. We also explored several initialization distributions, including uniform and normal distribution. We found that in case of our models, the truncated normal distribution, which bounds normally distributed variable from below and above, provides the best quality. Besides it, we noticed that applying dropout layer discussed in 2.1.5 significantly reduces overfitting of our model.

For entities and relations, we also experimented with initialization by pretrained embeddings. More specifically, we trained TransE, ConvE models and then utilised trained representations to initialize our model. In parallel, we initialized special token and positional embeddings with random values. As the dimensionality of the learnt TransE embeddings is lower than the dimensionality of our model's embeddings, we filled the remaining parts of embeddings with random values. Additionally, as the pretrained embeddings are in a wide range, which could harm the learning capability of our model, we experimented with scaling them by a constant factor. Nevertheless, during our experiments, we didn't notice any quality boost by using the above-discussed initialization techniques. Therefore, we decided to stick with random initialization approach, which we find simple and effective.

In our experiments, we also tested fixed-function initialization of positional embeddings, discussed in *Subsection* 2.5.3. In this case, the embeddings are fixed during the whole training procedure. We found that this initialization technique affects the quality of the trained models badly.

3.1.2. Sequence-to-sequence mapping

Regardless of the number of input tokens, several transformer layers are applied on top of all of them. In the default setting each transformer layer contains independent parameters. We also experimented with sharing all corresponding parameters between transformer layers, forming an architecture similar to ALBERT that was discussed in *Subsection* 2.5.5. We achieve similar quality of models in both settings. The parameter-sharing approach might be preferred in real applications as it has a few million less parameters. Nevertheless, more than half of the total number of parameters come from token embeddings.

Our experiments showed that the best performance is achieved when 6-12 transformer layers are applied. Importantly, each layer utilises multi-head attention mechanism discussed in *Subsection* 2.5.1. We found that at least 4 attention heads are needed to achieve the best quality of models. We also experimented with attention head dimension D_a and pointwise feed-forward layer dimension D_p. Our analysis showed the the best quality is attained when $2D_a = D_p = 512$. Lastly, we noticed that adding dropout layers before the components computing attention weights and before pointwise feed-forward layers, slightly reduces overfitting. Therefore, we include dropout layers in all our models.

3.1.3. Loss functions and model optimization

The goal of our context-free model is to restore the masked head/tail entity. To compute similarities between each entity $e_i \in E$ and the produced embedding p, we use dot product. More precisely, we compute

$$e_i \cdot p = \sum_{j=1}^{D} e_{ij} p_j \ ,$$

where $p = h_c$ if head entity was masked out and $p = t_c$ in case tail entity was masked out. As a result, a vector t is formed, such that t_i indicates a score of the i-th entity. Then, we apply softmax activation function on t to obtain a probability distribution $\tilde{t}$. Lastly, the cross-entropy loss function, discussed in *Subsection* 2.1.3, is computed between $\tilde{t}$ and a vector encoding an index of the masked head/tail entity. The computed loss is utilised to compute gradients of all model's parameters, including token embeddings. The optimization process is taken by Adam optimizer discussed in *Subsection* 2.1.4.

During our experiments, we found that several optimization details play a crucial role in boosting the quality of our models. First of all, we apply label smoothing discussed in *Subsection* 2.1.5. We find that it greatly reduces overfitting and in particular, setting label smoothing parameter $s \in (0, 1)$ to a high value $s > 0.5$ significantly increases the performance of our models on unseen samples. The exact optimal value of s is dataset-dependent, therefore it is finetuned for each experiment. The other important specific of our models is the gradient computation. On this point, the training process is more stable when softmax activation is computed along with cross entropy loss function, with the simplified formula. In our experiments, we noticed that it makes the gradient computation more precise and as a result the trained models converge faster. We also noticed that it impacts the final quality metrics measured on unseen samples.

We also experimented with other optimization variants. In particular, we discovered that an alternative approach is to replace softmax activation function with sigmoid activation defined using the formula

$$\sigma(x) = \frac{1}{1 + e^{-x}} \ .$$

In this setting, each entity is assigned a probability $\tilde{t} \in [0, 1]$ independently. In our experiments, we found that models trained in this way attain similar quality to when the softmax function is used. The other tested approach includes encoding all matching head/tail entities in one training sample. In this case, a vector encoding ground-truth entities contains multiple 1.0 values and the model is penalized by all of these entries at once. Nevertheless, we didn't notice any quality boost when using this approach.

3.1.4. Normalization layers

In our experiments, we also tested the impact of applying normalization layers discussed in *Subsection* 3.1.4. We found that including them in our models has a positive impact on the quality of our models. More specifically, we put normalization layers in 3 places, namely straight on top embeddings, after attention layers and after pointwise feed-forward layers. Including all of the above-mentioned layers have a strong positive impact on the final models' quality. Additionally, we noticed that using layer normalization over batch normalization is beneficial for our models. Lastly, we experimented with the placement of normalization layers inside transformer blocks, discussed in [25]. Nevertheless, we discovered that placing normalization layers in different parts of the transformer blocks doesn't have much impact on our models.

3.2. Adding context to the developed architecture

In the following section we will discuss the extensions developed to improve the context-free model. Particularly, we will focus on different approaches to utilise context of a graph representing training dataset. We reuse all of the components discussed in *Section* 3.1, including developed layers, overfitting prevention methods and loss functions. Nevertheless, we finetune parameters of each extended model separately as each of them has different characteristics. While this section covers only methods of putting additional context into the developed model, in *Section* 3.3 we discuss several strategies to train the extended models. Finally, we put everything together in *Section* 3.4, providing the most successful models.

3.2.1. Path-based context

The most natural approach to provide the context information to our model is to utilise nodes neighbouring with a given source entity. The simplest way of applying this idea is to add one random neighbour along with a relation connecting it with the source entity, forming a path $(e_h, r_h, e_p, r_t, e_t)$, where either e_h or e_t is masked out. An illustration presenting this approach is shown in *Figure* 3.3. In our experiments, we draw several millions of paths, each forming one sample with missing head and one sample with missing tail. We also find it beneficial for our models to randomly mask out intermediate entity e_p. It enforces the model not to memorize edges that are contained in constructed paths. Additionally, we experimented with paths longer than 2, nevertheless we didn't observe any quality boost by doing so.

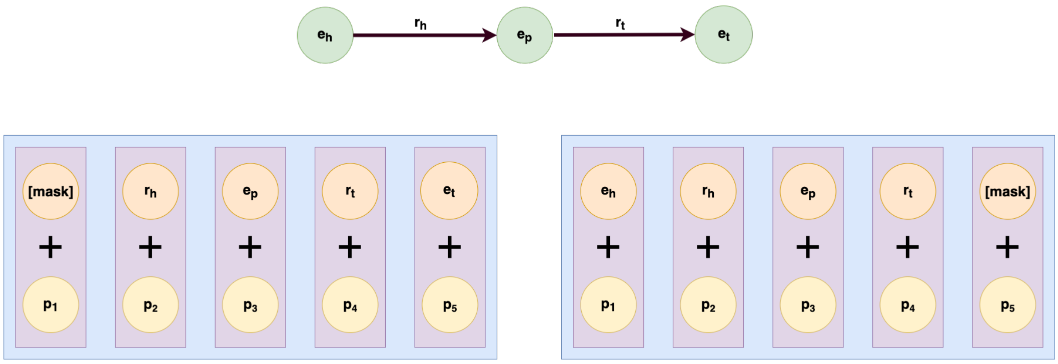


Figure 3.3: An illustration of how path-based context information is used during the training process. The top part of the figure presents a path of length 2 extracted from the knowledge graph, while the bottom part shows corresponding training samples. The bottom-left part illustrates a training sample with masked head entity. Similarly, the bottom-right part illustrates a training with masked tail entity. The entity e_p is randomly masked out with a probability defined by a hyperparameter.

3.2.2. Relation-based context

Another idea is to learn the model to predict a relation that connects given head and tail entities. This approach is illustrated in *Figure* 3.4. Intuitively, adding relation prediction task to optimize our model can help it in understanding different relations, leading the model to learn better representations. This knowledge can transfer to our final task of predicting a missing head/tail entity. As in this case the goal of the model is to restore a relation, similarities used for the loss computation are computed between the produced embedding and each relation $r_i \in R$.

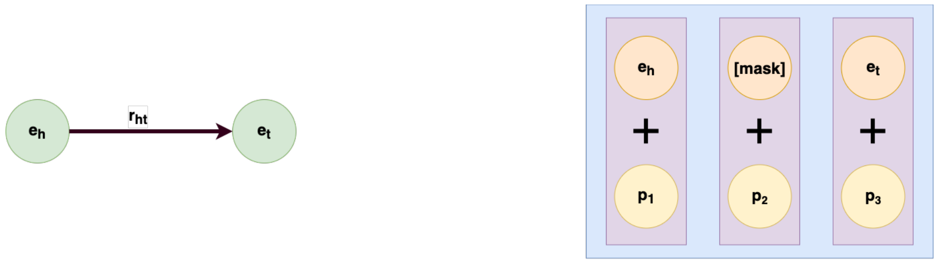


Figure 3.4: An example of how our models are learnt to predict relations. The left part of the figure shows the edge extracted from the knowledge graph, while the right side presents a training sample that corresponds to the extracted edge.

3.2.3. Neighbours-based context

We also experiment with adding a larger context to our model. More specifically, we encode input edges/output edges (or both) of the source entity. For each training sample, we use a fixed number of edges N. In case the source entity contains more than N neighbours, random N neighbours are sampled. On the other hand, if the source entity contains less than N neighbours, special tokens are put in the corresponding places of the input sequence. As the order of neighbours is not intended to impact the model's predictions, their positional embeddings are shared. The case when the source entity corresponds to the tail entity, while the head entity is masked out is shown in *Figure* 3.5. Similarly, the other case of tail entity masked out is illustrated in Figure 3.6.

During our experiments, we applied several modifications of adding neighbours-based context to our model. First of all, we randomly mask out the source entity to assure that the model does not memorize edges encoded in a given input sequence. Secondly, in case both input and output edges are included, we randomly mask out edges contained in one of this category. Lastly, we observed a positive impact of keeping the sampled neighbourhood of a given source entity fixed during the whole optimization process as well during the inference. In particular, it has a high impact on predictions of samples for which the source entity contains very large number of neighbours.

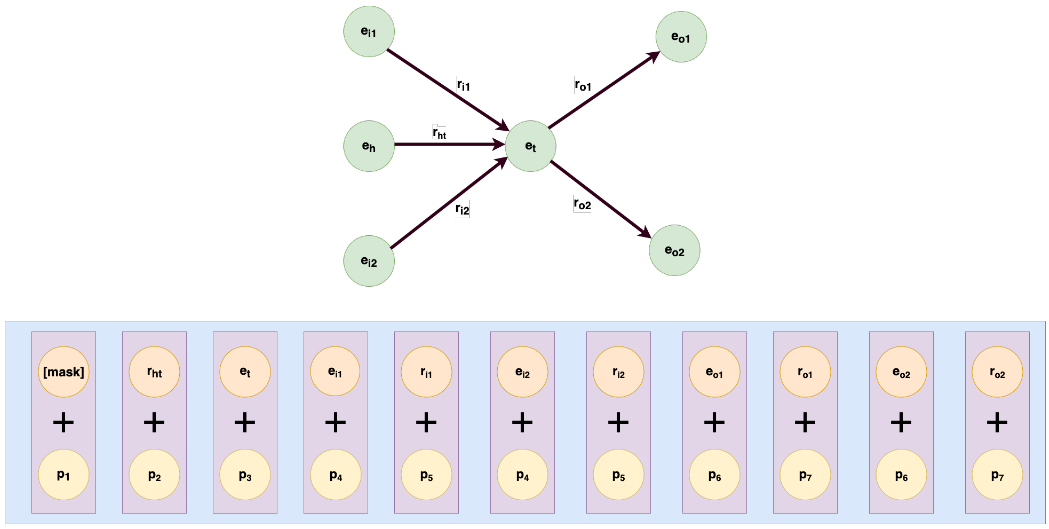


Figure 3.5: An example of how the context of input and output neighbours is utilised to produce a training sample with masked head entity. The top part of the figure presents a subgraph containing (e_h, r_{ht}, e_t) edge. The bottom part illustrates the subgraph encoded into input sequence taken by the model.

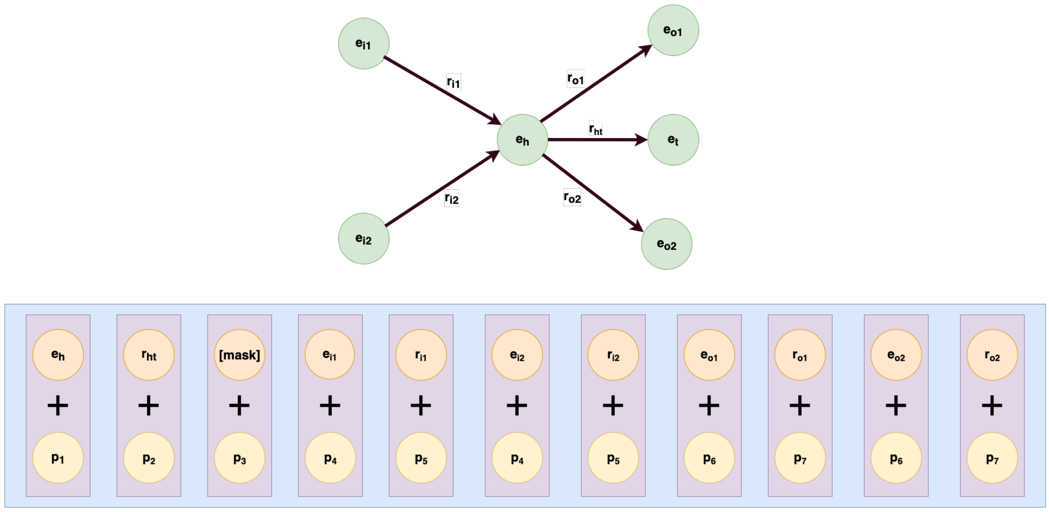


Figure 3.6: An illustration of how the context of input and output neighbours is used to form a training sample with masked tail entity. The top part of the figure shows a subgraph containing (e_h, r_{ht}, e_t) edge. The bottom part presents the subgraph encoded into input sequence taken by the model.

3.2.4. Similarity-based context

Our analysis of two benchmark datasets showed that many entities of a specific knowledge graph share common characteristics. In particular, many of them have common neighbours connected by the same relation. Inspired by this observation, we decided to collect similar entities and leverage these similarities during the optimization process of our model.

In order to formulate similarities, for each entity e_k we define a set of output relations $R_O(e_k) = \{r_1, \ldots, r_{M_k}\}$ (analogically a set of input relations) contained in the training dataset. We ignore the information of how many times a specific relation occurs in edges outcoming from e_k. We find two entities e_k, e_l similar if their sets of output edges $R_O(e_k)$ and $R_O(e_l)$ are similar. While there are many ways to formulate the similarity of sets, we use Jaccard index, which is defined using the formula

$$J_O(e_k, e_l) = \frac{|R_O(e_k) \cap R_O(e_l)|}{|R_O(e_k) \cup R_O(e_l)|}$$

Based on the above definition, we formulate the distance between two entities as

$$D_O(e_k, e_l) = 1 - J_O(e_k, e_l) \ .$$

For each entity e_k, we keep N entities that are the closest ones in the metric space defined by $D_O(e_k, e_l)$, forming $S_O(e_k)$ sets. To avoid the computation of similarities between each pair of entities explicitly, we use Ball Tree data structure that splits the space recursively in order to keep similar entities in neighbouring subspaces. Analogously, similar entities with respect to input edges are selected, forming $S_I(e_k)$ sets.

Now, we will focus on how we leverage $S_O(e_k)$ and $S_I(e_k)$ sets to add context information to our model. Our idea is to find edges that might be similar to a given, partially masked (e_h, r_{ht}, e_t) edge. In case the head entity e_h is masked out, we first extract entities similar to e_t according to the set $S_I(e_t)$. Then, we sample K edges $(e_{i(k)}, r_{ht}, e_{o(k)})$, such that $e_{o(k)} \in S_I(e_t)$. Intuitively, $e_{i(k)}$ might be a good candidate for being the masked head entity e_h. As a result, it makes sense to contain this information in the input sequence pushed to our model. The way of encoding this information is shown in *Figure* 3.7.

In case of the masked tail entity, the extraction of similar edges is analogous. The main difference is that the set $S_O(e_h)$ is used to extract searched entities. The other significant difference is that edges $(e_{i(k)}, r_{ht}, e_{o(k)})$ are samples with the $e_{i(k)} \in S_O(e_h)$ constraint. The discussed variant is illustrated in *Figure* 3.8.

During our experiments, we finetune the parameter controlling the number of similar entities pushed to the model. We also experimented with removing entities that are similar to the source entity from the input sequence. In this case, input sequences contain only entities that are candidates for being the masked out entity. Nevertheless, we did not observe any performance gains or losses by applying this modification. Lastly, as sampled context edges are permutation-invariant, we share their positional embeddings, what actually impacts the performance of our model positively.

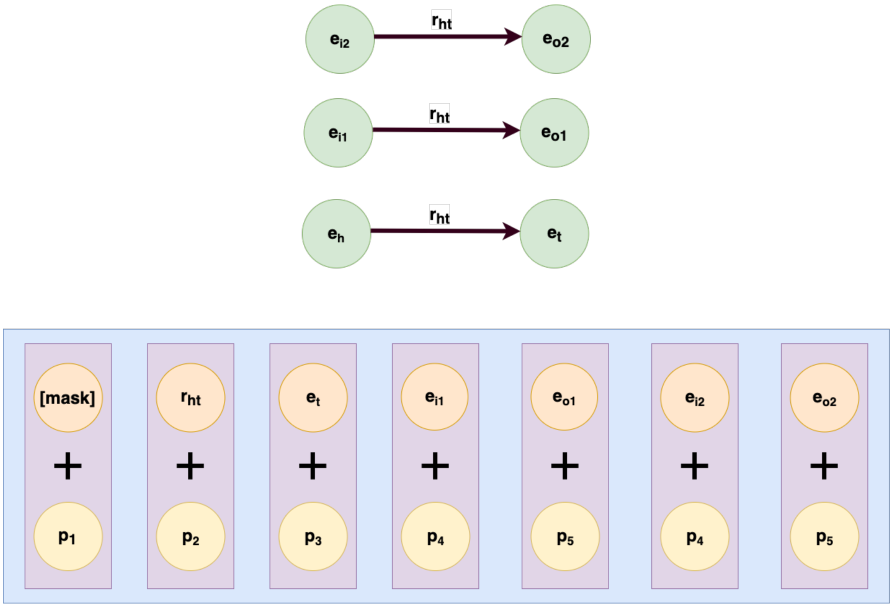


Figure 3.7: An example of how similar entities are utilised to form a training sample with a missing head entity. The top part of the figure presents a partially masked edge (e_h, r_{ht}, e_t) along with sampled edges, such that e_{o1}, e_{o2} entities are similar to e_t. The bottom part illustrates how this information is encoded into input sequence pushed to the model.

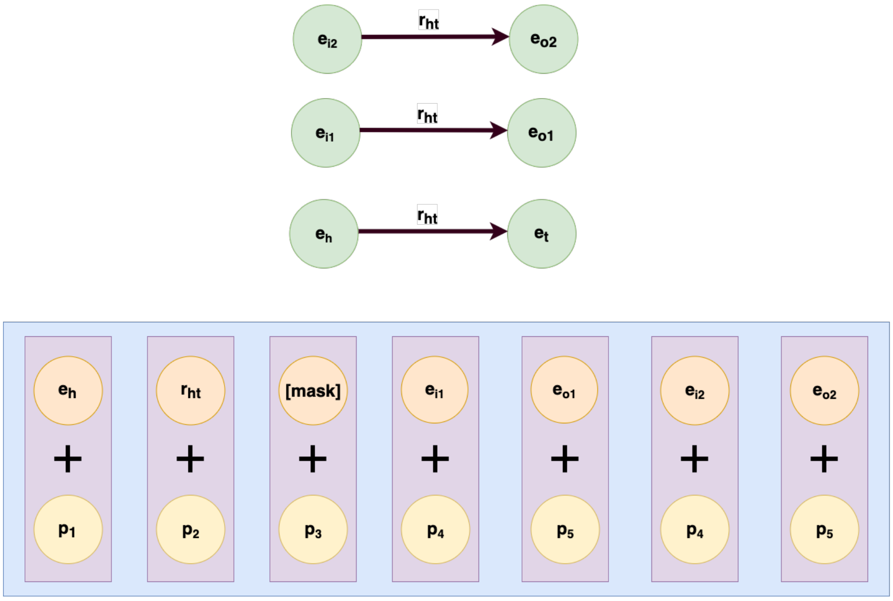


Figure 3.8: An illustration of how similar entities are used to produce a training sample with a missing tail entity. The top part of the figure illustrates a partially masked edge (e_h, r_{ht}, e_t) along with sampled edges, such that e_{i1}, e_{i2} entities are similar to e_h. The bottom part shows how these edges are encoded into input sequence pushed to the model.

3.3. Training strategies

There is nothing to prevent our models from being trained with multiple types of inputs, in particular those discussed in *Section* 3.2. In our experiments, we test 3 different training strategies to utilise various context types. Importantly, we keep positional embeddings of given triple's tokens fixed for all input sequences, regardless of the specific context that is used. In contrast, tokens corresponding to different contexts have disjoint positional embeddings. This allows the model to recognize different contexts, while being aware of which tokens correspond to a considered triple.

The first training strategy is to pretrain the model using different context types. More specifically, given a probability distribution defining the probabilities of drawing specific context types, at each training step one context type is sampled. Then, it is utilised to draw a batch of samples coming from the corresponding context's dataset. The whole pretraining process can be thought of interleaving input sequences containing various contexts. The probability distribution of selecting specific contexts is finetuned during the hyperparameter optimization process. After the pretraining procedure, the model is trained without context to tune its parameters to the final task of predicting a missing head/tail entity. The inference of the model on the the validation and test datasets is performed on raw triples, without any context included. Therefore, other tasks are used only to train better representations of entities and relations. We call this strategy of training the **context-sampling strategy**.

The other training strategy is to train the model with only one context type. In this setting, the model is not trained on raw triples at all. Importantly, the inference on validation and test datasets is also performed by constructing samples with a given context type. Intuitively, leveraging context information during the inference can positively impact the performance on unseen examples. In case the context information is sampled, we find it beneficial for our models to use the same context while doing the inference as during the training process. We call the above-discussed strategy of training the **context-only strategy**.

The last developed strategy of training is split into 2 phases. In the first phase, a separate transformer model is trained for each context. This is motivated by the fact that when multiple contexts are used at the same time, the model can learn to ignore some of them, particularly those that make up worse predictors. On the other hand, sharing parameters of transformer layers between input sequences coming from different context types, can encourage the model to memorize some parts of sequences. After each transformer model is trained, the training enters into the second phase, in which another transformer is put on top of the predicted embeddings. This allows the embeddings to exchange information and as a result improve their representations. After that, each embedding is used separately to compute a vector of similarities and the corresponding loss. Finally, all losses are summed up, forming the total loss. We call the presented training strategy the **separate-contexts strategy**.

3.4. Selected models

After testing various approaches and categories of models, we selected a few most representative ones that achieve the best performance. Importantly, each model has been finetuned independently to obtain the best quality possible. We call our first model that operates on raw edges without any context included, the **TransFree** model. The model that is pretrained to restore relations and missing head/tail entities of paths is called the **TransRP** model. In this case, the context-sampling training strategy is utilised. Going further, we call the model that is based on input and output neighbours, the **TransNIO** model. We find it beneficial to use the context-only training strategy in this case. Finally, we call the model with similarity-based context included, the **TransSim** model. Similarly, we use the context-only strategy to train it.

4. Experiments

As part of this thesis, we conducted several experiments applying our ideas presented in *Chapter* 3. Additionally, we compared the developed methods with competitive baseline models presented in *Section* 2.6. The first sections of this chapter describe the conducted experiments, while in the last section we present the obtained results.

4.1. Datasets

In the past, FB15K and WN18 datasets were used to evaluate the quality of knowledge graph completion models. After it was noticed that a large number of test triplets can be obtained by inverting training triplets, the **FB15K-237** and **WN18RR** datasets have been developed, reducing the above-mentioned problem. At this time, knowledge graph completion models are mainly evaluated on these two datasets. Therefore, we evaluate our models on FB15K-237 and WN18RR datasets.

The FB15K-237 dataset is a subset of a large open-source knowledge base, called Freebase. It contains relations between known people, movies, books, places and many others. The WN18RR dataset is a subset of WordNet, forming a large database of English words. Its graph contains lexical and semantic relations. While the FB15K-237 dataset contains several hundreds relations, the WN18RR dataset contains only 11. Additionally, the former one is much denser comparing the latter one. Therefore, the characteristics of both datasets are significantly different. The precise statistics of both datasets are presented in *Table* 4.1.

4.2. Metrics

In order to evaluate a model on a set of triples D, we utilise several ranking-based metrics for missing head and tail entities. Importantly, we do not use any triple contained in D during the evaluation of $d \in D$ i.e. the knowledge contained in other triples tested cannot be used to boost the predictions for a specific $d \in D$. The metrics are calculated for each triple contained in D and then averaged. Formally, let $(h, r, t) = \tilde{d} \in D$ denote a triple to be evaluated. To prepare a ranking for a missing head of $\tilde{d}$, we push a triple $([mask], r, t) = \tilde{d}_h \in D_h$ to a model. In case larger context

Statistic	FB15K-237	WN18RR
Entities	14,541	40,943
Relations	237	11
Training triples	272,115	86,835
Validation triples	17,535	3,034
Test triples	20,466	3,134

Table 4.1: Statistics of FB15K-237 and WN18RR datasets.

is used by the model, it is pushed along with $\tilde{d}_h$. The context includes only triples contained in the training dataset, particularly triples from the validation dataset are not used when evaluating the quality of the test dataset. As a result of this procedure, for each $\tilde{h} \in E$ we obtain a probability that $(\tilde{h}, r, t) \in G$. The obtained vector of probabilities forms a ranking, where $\tilde{h}_1$ takes a higher place than $\tilde{h}_2$ if and only if $P((\tilde{h}_1, r, t) \in G) > P((\tilde{h}_2, r, t) \in G)$. In case two triples have been assigned the same probability, they are put on the same place in the ranking. The discussed procedure forms an *initial ranking* $R_{\tilde{d},h}$ for $\tilde{d}_h$. The same procedure is repeated for the tail entity $\tilde{d}_t$, forming an *initial ranking* $R_{\tilde{d},t}$.

The *initial ranking* is postprocessed in order to obtain the *final ranking*. The first step involves removing triples that are contained in either training, validation or test dataset. This is known as a *filtered* setting, firstly proposed in [1] and widely adopted in other papers. Additionally, in case some probabilities outputted by the model correspond to other tokens than entities (e.g. relations), they are removed from the ranking. Finally, draws are resolved by putting $(\tilde{h}_1, r, t)$ higher in the ranking than $(\tilde{h}_2, r, t)$ if and only if $\sigma(\tilde{h}_1) < \sigma(\tilde{h}_2)$, where σ denotes a predefined order-determining function. Importantly, σ is fixed during the evaluation process and corresponds to the order of entities in the vocabulary. We determined that the same order is used when the baseline models have been evaluated by other authors. Performing the discussed steps on the given *initial ranking* $R_{\tilde{d},h}$ (analogically $R_{\tilde{d},t}$), forms the *final ranking* $\tilde{R}_{\tilde{d},h}$ (analogically $\tilde{R}_{\tilde{d},t}$) used to construct evaluation metrics.

Let us denote the position of the considered $\tilde{d}_h$ in the final ranking $\tilde{R}_{\tilde{d},h}$ (analogically $\tilde{R}_{\tilde{d},t}$) as $r(\tilde{d}_h)$ (analogically $r(\tilde{d}_t)$). The **Mean Rank (MR)** metric is defined by the formula

$$MR_h = \frac{1}{|D|} \sum_{\tilde{d}_h \in D} r(\tilde{d}_h) \ ,$$

which is simply a mean of rankings. Similarly, the **Mean Reciprocal Rank (MRR)** metric is defined by

$$MRR_h = \frac{1}{|D|} \sum_{\tilde{d}_h \in D} \frac{1}{r(\tilde{d}_h)} \ .$$

In contrast to the MR metric, the higher MRR metric denotes the better score. Additionally, the score given by the MRR metric grows exponentially with respect to the position in the ranking. As a result, improving the scores of triples that are already high in the ranking is promoted more, compared to improving the scores of triples that are low in the ranking. Lastly, the **Hits@10** metric is defined by the formula

$$Hits@10_h = \frac{1}{|D|} \sum_{\tilde{d}_h \in D} \mathbb{1}_{r(\tilde{d}_h) \leq 10} \ ,$$

where $\mathbb{1}_C$ is an indicator function that assigns 1 if and only if a condition C is satisfied and otherwise it assigns 0. Intuitively, the Hits@10 metric is the fraction of triples that were top 10 in the their rankings.

The above-defined metrics are calculated analogically for missing tail entities D_t, forming MR_t, MRR_t and $Hits@10_t$ metrics. Finally, the same metrics are calculated for all samples $D_a = D_h \cup D_t$, forming MR_a, MRR_a and $Hits@10_a$ metrics. While we use head-specific and tail-specific metrics to debug our models, we report only metrics for all samples, which we refer as $MR = MR_a$, $MRR = MRR_a$ and $Hits@10 = Hits@10_a$.

As we mentioned above, draws are resolved by the order-determining function σ. While this is a standard method at this time, in the recent past several researchers used another approach, causing the target triple to be often higher in the ranking. More specifically, as it was shown in [28], draws were resolved by putting the target triple first in case it draws with other entities. As a result, models putting the same probability for many entities performed very well, though their real quality was very poor. In particular, a model assigning the same probabilities to all entities achieves the perfect score in this setting. In our experiments, we often experienced this issue. Therefore, we decided to use order-determining function σ and compare our methods only with the models that have been evaluated or reevaluated using the same approach.

4.3. Methodology

Our models are trained on predefined training datasets of WN18RR and FB15K-237 knowledge bases. The predefined validation datasets are used to estimate the quality of models every few thousand steps. The total number of training steps depend on whether validation metrics indicate some progress. Specifically, in case the MRR metric on validation dataset is lower than the best one, 5 times in a row, the training procedure is stopped. The maximum number of possible training steps is set to 160,000, which corresponds to a few hundred epochs for both datasets. In practice, most of trained models converge after about 40,000 steps. After the training procedure, the model's state corresponding to the highest MRR value is chosen and saved.

We run the training procedure several times, each time sampling hyperparameters from the predefined set. In particular, for all models we finetune the initial learning rate along with decay rate, dropout rate, weight decay, label smoothing, activation function used in all layers, the dimensions of embeddings and layers, the number of attention heads in each layer and a standard deviation σ of initial parameters (truncated normal distribution is used for initialization). While the optimal values for most of the above-mentioned parameters are model-specific, we found that poor initialization leads the models to be stuck, making no progress. Therefore, learnable parameters of all models are initialized with $\sigma \in [0.01, 0.03]$. Additionally, we noticed that setting label smoothing s to a high value $s \in [0.7, 0.85]$ consistently provides better results. We also noticed a positive impact of applying dropout layers and weight decay. For all models, the optimal number of embeddings dimensions d_e was in $d_e \in [256, 512]$ range, while the optimal number of attention heads n_a lied in $n_a \in [4, 8]$ range. Furthermore, the optimal number of dimensions of attention heads and pointwise feed-forward layers lied in $[256, 512]$ and $[512, 1024]$ ranges, respectively. Lastly, we found that the best models use learning rate α in range $\alpha \in [0.0001, 0.0005]$ and linear decay with rate 0.0625 i.e. the learning rate of the last step is equal to $0.0625 \times \alpha$ and the learning rate of intermediate steps scales linearly.

The process of finding the best hyperparameters is repeated for each of the proposed models, forming separate categories. Afterwards, the best model for each category is chosen based on the MRR metric. In order to assess the quality of the chosen models, each of them is evaluated on the predefined test dataset. Additionally, we reproduce TransE, STransE and ConvE models, achieving similar results to those presented in other papers. Nevertheless, we compare our models with the results presented in original papers. In case, an original paper does not use the same evaluation protocol as the one discussed in *Section* 4.2, we rely on reevaluations performed by other researchers.

4.4. The obtained results

We have evaluated the developed models discussed in *Section* 3.4 against competitive baseline models discussed in *Section* 2.6. The full results are presented in *Table* 4.2. We find our approach competitive, especially when it comes to the MRR and $Hits$@10 metrics. In particular, in some cases our models are superior to all other models on these metrics. As we selected the models to maximize MRR, the competitive results on this metric were expected. We also obtained really good results on the $Hits$@10 metric, which correlates with the MRR metric. Lastly, we observe

Model	**FB15K-237**			**WN18RR**		
	MRR ↑	**MR ↓**	**Hits@10 ↑**	**MRR ↑**	**MR ↓**	**Hits@10 ↑**
TransE	0.294	357	0.465	0.226	**3384**	0.501
STransE	0.312	-	0.480	0.251	-	0.509
ConvE	0.325	244	0.501	0.430	4187	0.520
MINERVA	0.293	-	0.513	0.448	-	0.456
SACN	0.350	-	0.540	0.470	-	0.540
CompGCN	0.355	**197**	0.535	**0.479**	3533	0.546
TransFree	0.353	441	0.543	0.470	4670	**0.547**
TransRP	0.352	429	0.536	0.471	4792	0.545
TransNIO	**0.357**	380	0.542	0.473	4826	0.545
TransSim	0.354	309	**0.544**	0.471	4762	0.545

Table 4.2: Knowledge graph completion results on FB15K-237 and WN18RR test datasets. The up arrow next to the metric name means that higher values are better, while the down arrow depicts that lower values are better. The bold line after the CompGCN model separates the baselines from our models. The numbers that are bold depicts the best achieved results on a specific metric. Note that some authors have not evaluated their models on the MR metric.

that other models perform better on the MR metric, which is negatively correlated with the other two metrics. Nevertheless, the current approach utilised by most of researchers is to optimize the models on the MRR metric, while skipping the evaluations on the MR metric. This trend results from the fact that increasing the rank of entities that are far in the ranking, is not equally beneficial as increasing the rank of entities that are already high in the ranking. In other words, it is more useful to have less entities at the top of the ranking than having more entities in the middle of the ranking.

We also observed that our context-free model performs surprisingly well, while adding any context to it has little impact. Similar phenomenon can be observed when applying most graph neural networks on top of context-free methods. It is an open question whether additional context information is not useful in the problem of knowledge graph completion or the developed methods fail to extract it in the proper way.

5. Summary

In this thesis, we explored how transformed-based models can be applied to the knowledge graph completion problem. To reach our first milestone of outperforming context-free baseline methods, we developed an architecture operating on triples alone. We showed that it is superior to other methods in this category and presented the importance of the developed components, performing an extensive hyperparameters fine-tuning. In the next part of this thesis, we extended our model to include the context extracted from the graph representation of training data. We presented various approaches to apply this idea and conducted several experiments measuring the impact of each modification. Furthermore, we compared our models with context-free, reinforcement learning and graph neural networks approaches. The developed methods were superior to context-free and reinforcement learning models, while the best-performing graph neural network model achieved similar quality. We can conclude that transformer-based methods are competitive with the current state of the art methods, even when no context information is used or it is much smaller compared to other methods, which aggregate information from multi-hop neighbourhood.

5.1. Future work

Although transformers proved to provide a significant improvement over other methods, adding the context to the model boost the performance only slightly. In other words, the transformer architecture operating on triples alone provide a surprisingly high quality boost, while context-based transformer models only add a little bit of extra quality. The same pattern can be observed when applying graph convolutional networks on top of other methods. It is an open question whether it means that the context information is not so useful in the knowledge graph completion problem or the explored methods fail to extract it. One of the unexplored direction of future research is to combine transformer-based and graph-based methods. For instance, the CompGCN model could be used to aggregate information from the distant neighbourhood, while the transformer model could be applied on the aggregated embeddings. The other idea would be to stack a few transformers, one on top of each other. While this may sound like a graph neural network model, the transformers can be stacked in more custom ways, allowing layer-specific aggregations. Additionally, several extensions to the transformer architecture keep coming up and could be tried out to tackle the considered problem. One of recently developed pre-training methods include ELECTRA, discussed in *Subsection* 2.5.5. This method could be used to pretrain our model on long paths with some entities masked out.

5.2. Acknowledgments

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