

Embeddings in Natural Language Processing

Theory and Advances in Vector Representation of Meaning

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ABSTRACT

Embeddings have been one of the dominating buzzwords since the early 2010s for Natural Language Processing (NLP). Encoding information into a low-dimensional vector representation, which is easily integrable in modern machine learning algorithms, has played a central role in the development in NLP. Embedding techniques initially focused on words but the attention soon started to shift to other forms: from graph structures, such as knowledge bases, to other types of textual content, such as sentences and documents.

This book provides a high level synthesis of the main embedding techniques in NLP, in the broad sense. The book starts by explaining conventional word vector space models and word embeddings (e.g., Word2Vec and GloVe) and then moves to other types of embeddings, such as word sense, sentence and document, and graph embeddings. We also provide an overview on the status of the recent development in contextualized representations (e.g., ELMo, BERT) and explain their potential in NLP.

Throughout the book the reader can find both essential information for understanding a certain topic from scratch, and an in-breadth overview of the most successful techniques developed in the literature.

KEYWORDS

Natural Language Processing, Embeddings, Semantics

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CHAPTER 1

Introduction

Artificial Intelligence (AI) has undoubtedly been one of the most important buzzwords over the past years. The goal in AI is to design algorithms that transform computers into “intelligent” agents. By intelligence here we do not necessarily mean an extraordinary level of smartness shown by superhuman; it rather often involves very basic problems that humans solve very frequently in their day-to-day life. This can be as simple as recognizing faces in an image, driving a car, playing a board game, or reading (and understanding) an article in a newspaper. The intelligent behaviour exhibited by humans when “reading” is one of the main goals for a subfield of AI called Natural Language Processing (NLP). Natural language¹ is one of the most complex tools used by humans for a wide range of reasons, for instance to communicate with others, to express thoughts, feelings and ideas, to ask questions, or to give instructions. Therefore, it is crucial for computers to possess the ability to use the same tool in order to effectively interact with humans.

From one view, NLP can be divided into two broad subfields: Natural Language Understanding (**NLU**) and Natural Language Generation (**NLG**). NLU deals with understanding the meaning of human language, usually expressed as a piece of text.² For instance, when a Question Answering (QA³) system is asked “do penguins fly?”, the very first step is for it to understand the question, which in turn depends on the meaning of *penguin* and *fly*, and their composition. There are many challenges that make NLU an AI-hard problem:

- **Ambiguity.** One of the most important difficulties with human language lies in its ambiguous nature. Ambiguity can arise at different levels:
 - **Lexical ambiguity.** Words can simultaneously belong to multiple syntactic classes (parts of speech). For instance, *fly* can be a noun as well as a verb. But, more importantly, a word in a specific syntactic class can have multiple associated meanings (i.e., “senses”). For instance, the verb *fly* can refer to multiple meanings, including “travelling through the air” which is

¹Human language is referred to as “natural”, in contrast to programming or other artificial languages.

²The process of transcribing an utterance, i.e., converting speech to text, is the objective in Speech Processing, another subfield of AI.

³QA is one of the applications of NLP which deals with designing systems that automatically answer questions posed by humans in a natural language.

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the intended meaning in the above example, or “operating an airplane” as in “the pilot flew to Cuba” or “move quickly or suddenly” as in “he flew about the place”.⁴ We will talk more about “senses” and how to model them in Chapter 5.

- **Syntactic ambiguity.** A sentence could be parsed syntactically in multiple ways. For instance, in the sentence “I saw a man on the hill with binoculars”, we can attach *binoculars* to either *I* or to the *man*. As a result, different interpretations can be made depending on the choice of attachment. Syntactic ambiguity can also arise from conjunctions. For example, in “Avocado salad with cheese”, is cheese a part of salad or separate from that?
- **Metonymic ambiguity.** Metonymy is the substitution of a concept, phrase or word being meant with a semantically related one. For instance, in “Cambridge voted to stay in the EU”, it is definitely the people of Cambridge who voted and not the city itself.
- **Anaphoric ambiguity.** This type of ambiguity concerns the interpretation of pronouns. For instance, in “I have a laptop but recently bought a new one. I am going to give it away.”, what does *it* refer to?
- **Common sense knowledge.** Addressing many of the ambiguities requires something that is not explicitly encoded in the context; it needs world knowledge or some reasoning. For instance, in the example for anaphoric ambiguity it is easy for a person with background knowledge to attach *it* to the old laptop. Referential ambiguities that need background knowledge for resolution is the target for Winograd Schema Challenge [Levesque et al., 2012] which is deemed to be alternative to the Turing Test for machine intelligence. Similarly, it would be easy for humans to identify the intended meaning of *mouse* in “I ordered a mouse from Amazon” given their background knowledge from the marketplace.
- **Figurative language.** Idioms such as “fingers crossed” and “all ears” and sarcasm are forms of figurative language that are extensively used by humans in both conversational and written form. Given that the meaning behind these expressions are not usually directly achievable from their constituent words, they pose a serious challenge for language understanding algorithms.

Many of the applications in NLP require addressing one or more of the above challenges. For instance, Machine Translation often requires extensive handling of different types of ambiguity to be able to transform meaning from a language to another one, with both having their own implicit ambiguities. Similarly, Question Answering not only has to deal with ambiguities but also sometimes requires a grasp of

⁴Definitions from WordNet (more about this lexical resource in Chapter 2). WordNet 3.0 lists 14 meanings (senses) for the verb *fly*.

background common sense knowledge for making inference about facts and answering questions. Also, there are many NLP tasks that are targeted at the above research challenges in order to pinpoint the research efforts to specific areas that need more attention. For instance, Word Sense Disambiguation deals with identifying the intended meaning of a word in a given context, coreference resolution is focused on resolving anaphoric ambiguity, and semantic similarity measurement measure the ability of models in modeling the semantics of words or longer pieces of texts.

NLG can be considered as the opposite of NLU: the goal is for a computer to generate text, or in other words to “talk” to humans through natural language, either to verbalise an idea or meaning, or to provide a response. NLG is difficult for several reasons including massive vocabulary size from which the computer has to pick specific words to convey the idea, the properties of natural language that allow dynamic word order, and for the need for fluency and accordance with grammar of the target language. Many of the NLP applications involve generation, such as Question Answering, text summarization, and conversational AI.

Semantic representation, the topic of this book, lies at the core of most NLP models, from understanding to generation. Therefore, the inherent semantic representation is a crucial playmaker in the performance of downstream applications. In the following sections we will talk more about semantic representation. Most of the works discussed in this book deal with the English language. Therefore, some conclusions may or may not generalize to other types of language. While acknowledging this limitation, we have also attempted to refer to other languages and their challenges in some chapters and sections, to let the reader better understand the generalization of some of the points addressed in the book.

1.1 SEMANTIC REPRESENTATION

Imagine the word “desk”. When stored on a computer, this word is nothing but a sequence of four characters “d”, “e”, “s”, and “k”. But computers only understand zeros and ones. Hence, each character has to be stored as a pattern of bits. The number of bits depends on the encoding. For instance, the extended ASCII needs 8 bits for storing each character. Therefore, the word “desk” is *represented* as a sequence of 32 zeros and ones according to this encoding.⁵. A five-character word, such as “table”, will get a 40-bit long representation.⁶. This approach is not a favorable way of representing the semantics of words, due to the following limitations:

1. The representation cannot incorporate semantic information of words, e.g., the semantically similar words “table” and “desk” (or even synonymous words

⁵ASCII encoding for “desk”: 01100100 01100101 01110011 01101011

⁶ASCII encoding for “table”: 01110100 01100001 01100010 01101100 01100101

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{basket:1,	desk	[] [] [] [] [] [] [] [] [] []
fork:2,	desks	[] [] [] [] [] [] [] [] [] []
desk:3,	plate	[] [] [] [] [] [] [] [] [] []
cloud:4,		[] [] [] [] [] [] [] [] [] []
plate:5,		[] [] [] [] [] [] [] [] [] []
rabbit:6,		[] [] [] [] [] [] [] [] [] []
desks:7,		[] [] [] [] [] [] [] [] [] []
tree:8,		[] [] [] [] [] [] [] [] [] []
table:9,		[] [] [] [] [] [] [] [] [] []
lion:10}	table	[] [] [] [] [] [] [] [] [] []

Figure 1.1: A toy vocabulary of ten words with their corresponding one-hot representations.

“noon” and “midday”) will have totally different representations. We are ideally looking for a representation that can encode semantics of words.

2. The representation is character-wise. Therefore, the size of the representation depends on the length of the words (number of characters they have). The variable size is an unwanted property which further complicates the comparison of representations of different words. In fact, it is not straightforward to integrate these variable-sized representations into machine learning models, which generally “understand” feature-based representations.

1.2 ONE-HOT REPRESENTATION

We can address the variable-size issue of character-level representations by directly representing words rather than characters. Imagine an ASCII-like encoding that instead of mapping characters to 8-bit binary representations, it maps words to distinct fixed-sized patterns of zeros and ones. This is the idea behind one-hot representation which is the simplest form of word representation. Assume we have 100 words in a vocabulary and we would like to have them as one-hot representations. First, we associate an index (between 1 to 100) to each word. Then, each word is represented as a 100-dimension array-like representation, in which all the dimensions are zero except for the one corresponding to its index, which is set to one (therefore the name “one-hot” encoding). Note that, one-hot encoding is different from our earlier ASCII-like representation in that it is highly sparse, i.e., it contains only one single 1 and the rest are zero. Figure 1.1 shows a toy example with a vocabulary of 10 words along with their indices (left) and one-hot representations (right). Despite its simplicity, one-hot encoding constructs the foundations for more flexible Vector Space Models (to be elaborated in the next section).

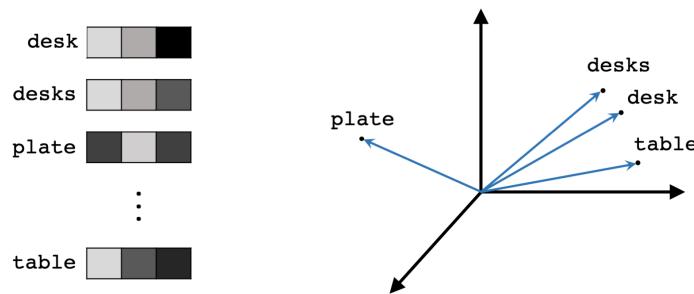


Figure 1.2: Representing words in the example in Figure 1.1 in 3-dimensional continuous vector space. Note the continuous embeddings in the vectors (compared to binary values in Figure 1.1) and the notion of similarity between “desk”, “desks”, and “table”.

One-hot representation partly addresses the second limitation discussed above. However, it still suffers from the first limitation: each word is assigned with a different representation and there is no notion of “similarity” between these representations. Using this representation, it is not possible to encode the conceptual similarity between “noon” and “midday”. Even worse, the two similar looking words such as “desk” and “desks” (which would have similar string-based representations) are assigned with completely different representations.

Moreover, as one can guess from Figure 1.1, the size of one-hot representations grow with the number of words in the vocabulary. In a typical vocabulary, we should expect hundreds of thousands of words. Representing each word using one-hot representation is definitely too storage-intensive and would make the processing difficult (see dimensionality reduction in Chapter 3).

1.3 VECTOR SPACE MODELS

Vector Space Model (VSM), first proposed by Salton et al. [1975], provides a solution to the limitations of one-hot representation. In this model, objects are represented as vectors in an imaginary multi-dimensional continuous space. In NLP, the space is usually referred to as the *semantic space* and the representation of the objects are called **distributed representation**. Objects can be words, documents, sentences, concepts or entities, or any other semantic carrying item between two of which we can define the notion of similarity. In this chapter, we mostly focus on words because they are one of the most widespread applications of VSM in NLP.⁷

⁷Throughout this book, unless we explicitly specify, by representation we often mean a word representation, given that most research in VSM has been around word representation.

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Figure 1.2 shows a simple 3-dimensional semantic space that represents four words with their corresponding vectors. In fact, one-hot representation is a specific type of a distributed representation in which each word is represented as a vector along with one of the axes in the semantic space (the semantic space needs to have n dimensions where n is the number of words in the vocabulary). Moving from the *local* and discrete nature of one-hot representation to *distributed* and continuous vector spaces brings about multiple advantages. Most importantly, it introduces the notion of similarity: the similarity of two words (vectors) can be measured by their distance in the space. Moreover, many more words can fit into a low dimensional space; hence, it can potentially address the size issue of one-hot encoding: a large vocabulary of size m can fit in an n -dimensional vector space, where $n \ll m$.

Figure 1.3 provides a more realistic example with many more words in a 2-dimensional space. Usually, semantic spaces have hundreds of dimensions. Given it is not possible to imagine such high dimensionalities, we usually leverage dimensionality reduction techniques (cf. Chapter 3) to reduce the size of the semantic space to two or three for visualization purposes. In Chapter 2, we will describe the process of learning distributed word representations and their variants.

VSM has been one of the most successful ideas in NLP; it is undoubtedly the prevalent solution for representing semantics, also supported by research in conceptual spaces for cognitive knowledge representation [Landauer and Dumais, 1997, Gärdenfors, 2004]. According to cognitive representation, humans characterize objects with respect to the features they possess. Brain models similarities between objects according to the similarities between their features.

Distributed representations have established their effectiveness in NLP tasks such as information extraction [Laender et al., 2002], semantic role labeling [Erk, 2007], word similarity [Radinsky et al., 2011], word sense disambiguation [Navigli, 2009] or spelling correction [Jones and Martin, 1997], *inter alia*. The process of constructing distributed representations has undergone a long history of development in the past few decades but their constitutional property has remained unchanged: distance in the vector space denotes a notion of semantic similarity. It is important to note that distributed representation is not only limited to words; it can be applied to any other type of concepts or textual forms, such as word senses, entities, sentences, documents, or word senses (all to be covered in this book). Turney and Pantel [2010] provide a comprehensive survey of conventional VSM techniques in NLP.

1.4 THE EVOLUTION PATH OF REPRESENTATIONS

Vector Space Model [Salton et al., 1975] was initially centred around modeling documents in information retrieval systems. Despite being simplistic in nature, the approach proved very successful since its introduction. This persuaded researchers,

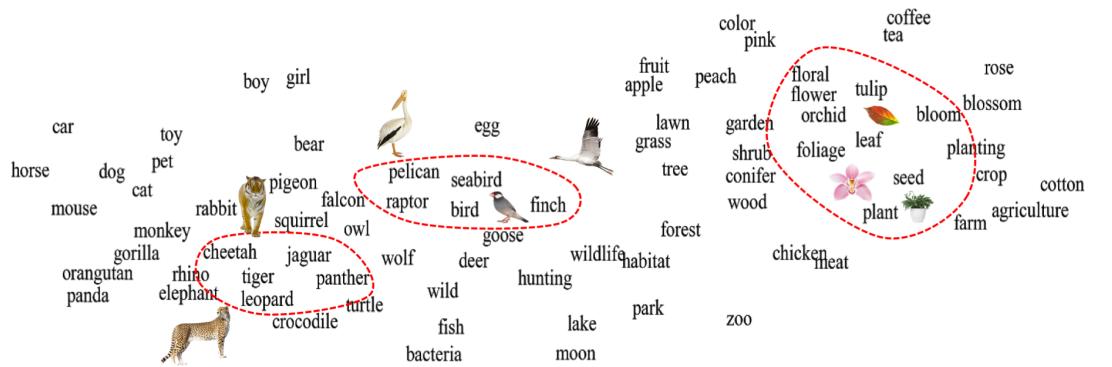


Figure 1.3: Subset of a sample word vector space reduced to two dimensions using t-SNE [Maaten and Hinton, 2008]. In a semantic space, words with similar meanings tend to appear in the proximity of each other, as highlighted by these word clusters (delimited by the red dashed lines) associated with *big cats*, *birds* and *plants*.

such as Deerwester et al. [1990], to extend the model from documents to other forms, particularly words. The compatibility of vector-based representation with conventional and modern machine learning and deep learning has significantly helped the model to prevail as the dominant representation approach for the past few decades.

The *distributional hypothesis* [Harris, 1954, Firth, 1957], i.e., words that occur in the same contexts tend to have similar meanings, has been the foundation of automatically constructing word VSM. However, the interpretation of the hypothesis and the way of collecting “similarity” clues and constructing the space have gone under enormous changes. Earlier approaches were based on collecting word statistics, usually in terms of occurrence and co-occurrence frequency. Hence, they are usually referred to as *count-based* techniques (Section 3.1). These representations are often large and needed some sort of dimensionality reduction (Section 3.1.2).

The deep learning tsunami hit the shores of NLP around 2011. Word2vec was one of the massive waves from this tsunami and once again accelerated the research in semantic representation. Despite not being “deep”, the model was a very efficient way of constructing compact vector representations, by leveraging (shallow) neural networks. Since then, the term “embedding” almost replaced “representation” and dominated the field of lexical semantics. The fresh blood in veins of lexical semantics resulted in dozens of specialised embedding techniques emerged, such as sense embedding (Chapter 5), retrofitted embeddings (Section 3.4), and cross-lingual embeddings (Section 3.5), many of which are based on Word2vec. This also accelerated research in other areas of representation, such as embeddings of nodes and relations in structured knowledge resources, such as semantic networks.

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Word embeddings proved to be potent keepers of semantic; their integration in various benchmarks resulted in considerable improvements Baroni et al. [2014]. However, they still suffered from a major limitation: they fall short of modeling the dynamic nature of words. Words can exhibit different syntactic and semantic properties depending on the context in which they appear. For instance, the term *mouse* can refer to unrelated meanings (rodent and computer device) depending on the context in which it appears. Word embeddings are static in nature; the embedding for *mouse* is unchanged across these contexts.

The latest wave is indeed the so-called contextualized representation. The approach is aimed at addressing the static nature of word embeddings by allowing the embedding to adapt itself to the context in which it has appeared. Differently from conventional word embeddings, the input to these models is not words in isolation, but words along with their contexts. Contextualized representations are currently dominating almost all standard NLP benchmarks. Also, the field is rapidly evolving, with several major advancements in the past few years. Chapter 6 talks about this new branch of representation.

1.5 COVERAGE OF THE BOOK

This book should be of interest to all AI researchers who work with natural language, especially those who are interested in semantics. Our goal with writing this book is to introduce the topic of semantic representation to those who are new to the area, and to provide a broader perspective to those who are already familiar with the area with a quick overview of recent developments and the state of the art in various branches. The book synthesizes the diverse literature on semantic representation and provides a high level introduction to major semantic embedding models.

We note that in our overview of various techniques, we provide details only to that depth that are necessary to sketch the general shape of the field and to provide a hint on how the research problem was approached. In these cases we also provide with relevant references so that the reader can investigate a specific sub-area on their own. We hope this book can bring fresh researchers and practitioners up to speed on the recent developments in the field, while pointing out open problems and areas for further exploration.

1.6 OUTLINE

The book is split into nine chapters as follows:

1. In Chapter 2, we provide some **background knowledge** on the fundamentals of NLP and machine learning applied to language problems. Then, we briefly

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describe some of the main knowledge resources that are commonly used in lexical semantics.

2. Chapter 3 discusses **word representations**, starting from a brief overview of conventional count-based models and continuing with the more recent predictive and character-based embeddings. We also describe in the same chapter some of the techniques for specialising embeddings, such as knowledge-enhanced and cross-lingual word embeddings, and common evaluation methods for word representations.
3. Chapter 4 covers various techniques for embedding structural knowledge resources, in particular semantic **graphs**. We will overview major recent methods for embedding nodes and edges of graphs and conclude with their applications and evaluation.
4. In Chapter 5 we focus on the representation of individual meanings of words, i.e., **word senses**. The two classes of sense representation (unsupervised and knowledge-based) are discussed, followed by evaluation techniques for this type of representation.
5. Chapter 6 is about the recent branch of **contextualized embeddings**. In this chapter, we first explain the need for such embeddings and then describe the prominent models and how they are tied with language models. We also cover in the same chapter some of the efforts to explain and analyze the effectiveness of contextualized models.
6. Chapter 7 goes beyond the level of words, and describes how **sentences and documents** can be encoded into vectorial representations. We cover some of the prominent supervised and unsupervised techniques and discuss the applications and evaluation methods for these representations.
7. Chapter 8 explains some of the **ethical issues** and inherent biases in word embeddings, which have been the topic of discussion recently. The chapter also covers some of the proposals for debiasing word embeddings.
8. Finally, in Chapter 9 we present the **concluding remarks and open research challenges**.

CHAPTER 2

Background

2.1 NATURAL LANGUAGE PROCESSING FUNDAMENTALS

Natural Language Processing (NLP) lies at the intersection of linguistics and computer science. In this section we cover some fundamental topics in linguistics and NLP which will be recurrent in most of the chapters. While the coverage of these topics will be quite shallow, this will give the reader a basic understanding which should be enough to understand the rest of the book.

2.1.1 LINGUISTIC FUNDAMENTALS

Linguistics, as an area of study, comprises many subfields; for instance, phonetics, phonology, lexicography, psycholinguistics, and discourse. While in this book we will not cover these topics in-depth, we would recommend [Bender \[2013\]](#), a book from this editorial, which covers the most important aspects of linguistics directly related to natural language processing. In the following, we provide a brief overview of three major fields of study in linguistics that are related to the topic of this book.

Syntax. Syntax deals with the structures of sentences. It shows the rules and principles that specify the order in which words are put together in a sentence in a given language. For instance, syntax of the English language denotes that sentences in this language should have the subject–verb–object (SVO) order (where the subject comes first, followed by the verb, and then the object) whereas syntax for Farsi or Korean languages generally follows the SOV order. Grammar is a more general concept which involves syntax but also other rules governing a language, such as morphology.

Morphology. Morphology deals with the structure of words and studies their constituent parts (roots, stems, prefixes and suffixes). It shows how words are formed and how they are related to each other in a language. A language like Farsi is morphologically rich, given that for instance a verb in this language can take many inflected forms whereas languages such as English are less morphologically diverse.

Semantics. Semantics is the area of linguistics that studies meaning. This is clearly the area which is the central focus of this book. In fact, what we generally expect from an embedding is a machine-readable representation that encodes the semantics (or

meaning) of a word, a sentence, etc. While there are different branches of semantics, this book mainly deals with lexical semantics, which is the branch that studies word meaning. Then there are also a few chapters (especially Chapter 7) where compositional semantics, i.e. how to combine smaller pieces into larger units such as sentences or documents, come into play.

2.1.2 LANGUAGE MODELS

Language Models (LM) are intended to distinguish grammatical from ungrammatical sequences in a specified language [Chomsky, 1957]. In other words, given a phrase or a sentence in a language, a LM has to identify if it is fluent or plausible according to the grammar of that language or not. For instance, a language model is expected to identify “high air pollution” as a fluent sequence in English that accords with its grammar, whereas “high pollution air” as unfluent or ungrammatical.

The statistical approach to language modeling usually makes an n -th order Markov assumption and estimates the probability of a given sequence based on the statistics of n -gram frequencies in a large text corpus, usually followed by a smoothing. Statistical LM is one of the major components of Statistical Machine Translation (SMT) which were the prominent machine translation technique before the introduction of Neural Machine Translation (NMT). The LM component of SMT is responsible for generating “grammatical” translations in the target language. Roughly speaking, among a set of candidate translations, the LM unit picks the one that is more fluent in the target language.

Statistical LM suffers from data sparsity given that the number of possible n -grams in a language grows exponentially with respect to the vocabulary size and sequence length, a phenomenon also known as the curse of dimensionality. Neural models address the sparsity issue of count-based LMs by moving from the local one-hot representation of words to a continuous distributed one (see Section 3.2). To this end, during sequence modeling each word is represented as a continuous vector, incorporating the notion of vector space similarity. The continuous representation of words pushes the language model to learn grammatical and semantic *patterns* instead of exact sequences of words. This in turn results in a smooth modeling that allows the NLM to assign high probabilities to unobserved sequences based on similar patterns (semantic and functional similarity) that were observed during training.

In this manner, language modeling has largely benefited from distributed representations. Interestingly, the benefit has recently turned out to be mutual. The application of LM has vastly expanded from machine translation and generation-oriented tasks to representation learning. In fact, most of the recent successful word representation techniques are closely tied with language modeling.

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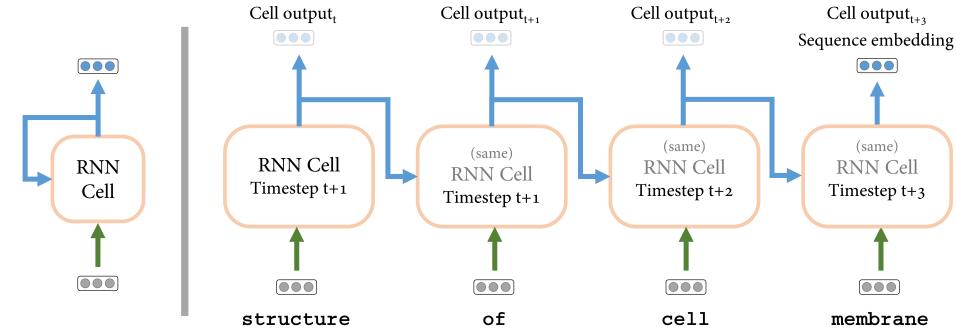


Figure 2.1: Left: RNNs have a loop that allows the network to “remember” the past words in the sequence. The loop is unrolled on the right side, illustrating how the RNN functions. Note that the same RNN cell is applied in different time steps to the words in the sequence.

It is shown by different researchers that to fulfil the simple objective of predicting the next word (or a set of missing words), language models are forced to encode complex syntactic and semantic information [Goldberg, 2019, Jawahar et al., 2019]. Owing to this, the recent neural language models that are usually trained on massive amounts of text have been the dominating approach for semantic representation. In Chapter 6 we will discuss contextualized representations and explain their close ties with language models. In the following section we provide more details on neural networks applied to NLP, for language models and other tasks.

2.2 DEEP LEARNING FOR NLP

In early 90’s, a revolution in the field of NLP gradually led to a shift from Chomskyan linguistic theories to Machine Learning (ML). Since then, ML has empowered many applications in NLP. For almost two decades, statistical ML techniques were the favourite solution for many NLP tasks and dominated most of the benchmarks. The general approach was to train shallow models on usually high dimensional and sparse hand-crafted features. Classification-based NLP tasks, such as sentiment analysis, topic categorization, and word sense disambiguation, were conventionally approached using classifiers such as Support Vector Machines (SVM) and Maximum Entropy (MaxEnt), whereas Conditional Random Field (CRF) was the predominant solution to structured prediction tasks, e.g., Named Entity Recognition (NER) and chunking.

In the past decade, a new revolution has taken place. Upon a highly successful introduction in Machine Vision, deep learning was like a huge tsunami that hit the

shores of NLP, and has so far dominated the field. A seminal work in this branch is that of [Collobert et al. \[2011\]](#) who showed that a simple neural network, with no explicit intervention during training, can outperform feature-based techniques across several tasks, such as NER and Part-of-Speech tagging. Word2vec [[Mikolov et al., 2013a](#)] was probably another big wave of this tsunami whose impact is still being felt today. Again, a simple neural network was shown to be highly efficient and effective in capturing semantics of words compared to computationally expensive statistical techniques which also required an extra step of dimensionality reductions. In Chapter 3 we will elaborate on Word2vec.

Another impactful deep learning technique that revolutionised many of the NLP systems at the time is the Long Short-Term Memory (LSTM) network (Section 2.2.2). Until very recently, LSTMs were the optimal solution for encoding sequences into dense continuous representations, with several desirable properties that were lacking in the previous models, such as their ability to capture word order and long-distance dependencies. Prior to LSTMs, sentence-level representation was either limited to simplistic models such as bag of words or had to resort to local word orderings, such as n -grams. Convolutional neural networks (CNNs) grew in parallel to LSTMs and showed powerful in tasks such as sentiment analysis and topic categorization. However, they did not attain the popularity of LSTMs since they cannot capture word order on their own. For a comprehensive overview of neural networks and their application to NLP, the reader might refer to the book of [Goldberg \[2017\]](#).

2.2.1 SEQUENCE ENCODING

Unlike words, it is not feasible to pre-train embeddings for all word sequences (phrases, sentences, etc) in a natural language, given that the number of possible sequences can be infinite. Therefore, the representation for a text sequence is often computed as the combination of its words' representations. Chapter 7 talks about the representation of longer pieces of texts, such as sentences and documents.

The most trivial “combination” strategy is called the bag of words (BoW) model: the representation for the sequence is obtained by averaging the representations of its individual words. In other words, a set of words are represented as their *centroid* point in the vector space. An important issue with the BoW representation is that all words play equal role in the final representation of the sequence (since an unweighted average). However, it is natural to expect that some words in the sequence might be more central to its semantics. There are variations of BoW that assign weights to words while combining, based on TF-IDF or other information measuring schemes. Additionally, there is another important issue with the BoW representation that still remains unaddressed. These representation are called bag of words because they ignore the order of words while “combining”, which can be crucial in terms of se-

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mantics. For instance, the semantically different sequences “rain stopped the match” and “match stopped the rain” (and many other ungrammatical sequences constructed using these words) will have an identical BoW representation.

Recurrent Neural Networks (RNN) have successfully come into play to address the above issues in NLP. RNNs are a special type of neural architecture that are characterized by their recurrence: unlike feedforward networks (such as fully connected and convolutional neural networks), RNNs have feedback loops allowing the network to exhibit temporal dynamic behavior and “remember the past”. Feedforward networks often receive the input at once; hence, unless some additional measure is taken, they have no means of capturing the order in sequential data.¹.

Figure 2.1 shows a high-level illustration of a simple recurrent neural network. The same RNN cell receives the input word embeddings in a sequence of timesteps. The output for each timestep is computed by combining the current input and the output from the previous timestep. This output (vector) will be passed as an additional input to the next timestep and this recurrence repeats until end of the sequence is reached. The simplest form of combination can be to multiply each of these vectors to their corresponding weight matrices and then add them to construct the output for the current timestep. In this way, RNNs can “remember” the past, something which is crucial for accurate encoding of semantics.

$$h_t = f(Wx_t + Uh_{t-1} + b_o) \quad (2.1)$$

where $f()$ is an activation function of choice (e.g., sigmoid), x_t is the input embedding at time t (for the t^{th} word) and h_{t-1} is the output (embedding) from the previous timestep ($t - 1$). b is the bias term and W and U are the weight matrices to be learned during the training. The final h embedding (for the last timestep, or after reading the last word in the sequence) can be taken as the embedding for the sequence.

2.2.2 RECURRENT NEURAL NETWORKS

Since their adoption, recurrent neural networks have been prominent in NLP for a number of tasks. In this section we provide details on different variants and models.

RNN variants

In the following we explain different variants to encode sequences (in particular word sequences) using RNNs.

Bidirectional RNN A widely-used extension of RNN is the Bidirectional RNN (BiRNN). In this case, the input sequence is fed from beginning to end and also

¹We will see in Section 6.2 how a feedforward network, called the Transformer, can be also effectively used for sequence encoding

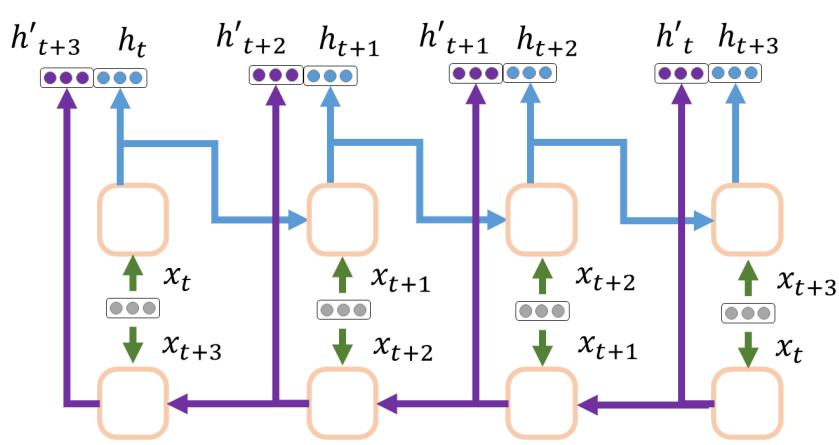


Figure 2.2: Bidirectional RNN. The text sequence is fed to the network in both directions to allow each timestep to have access to future inputs.

from end to the beginning. This would allow a cell state to have access to “future” timesteps, i.e., the next words in the input sequence. Figure 2.2 illustrates the architecture of BiRNN. The resulting h vector for BiRNNs is formed by combining (e.g., concatenating) the output vectors h and h' from the two directions. It is not difficult to think of cases in which having “future” context might help. For instance, in the sentence “cell is the biological unit of all living organisms”, unless we have seen words that are to the right of the ambiguous word *cell*, it is impossible to have a clear understanding of the intended meaning of this word. BiRNNs are shown to be beneficial to many NLP tasks, such as Machine Translation.

Stacked RNNs It is also possible to stack multiple layers of RNN on top of each other, a setting which has shown to help in some tasks. For instance, Google Translate makes use of a stack of 8 LSTM layers to encode and another 8 to decode the sequence in source and target languages [Wu et al., 2016]. In the case of stacked RNN, in the intermediate layers, instead of taking the final h_t as the output, all h_t values from different timesteps are passed in the same order, as input to the subsequent RNN cell (next layer).

Vanishing gradient problem. Backpropagation is the most widely used algorithm for training neural networks. To minimize the loss function, backpropagation computes the gradient of the loss function with respect to the weights; hence a *gradient-based* procedure. In order to avoid redundant calculations, the gradients are calculated using the chain rule from the last layer (where the loss is

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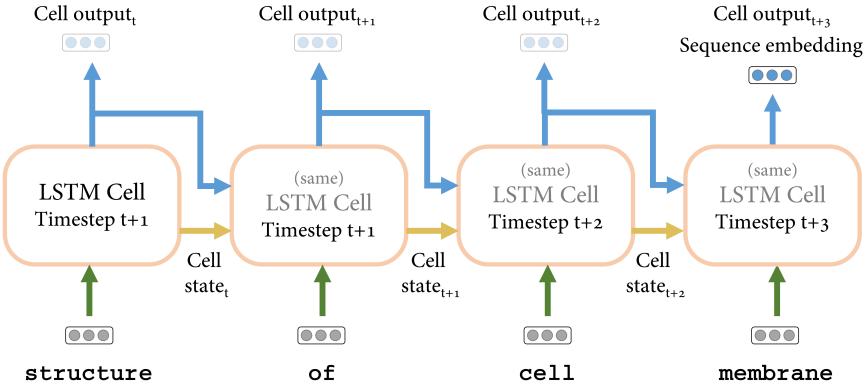


Figure 2.3: Long Short-Term Memory (LSTM) features a “carry track” that transfers the cell state across timesteps, allowing long-term dependencies to be captured.

computed) iterating backward. Therefore, the gradient value can vanish^a quickly as we move backwards towards the “front” layers. This difficulty is usually referred to as vanishing gradient problem and can make it impossible to train deep neural networks. The impact of vanishing gradient in recurrent networks (which are deep with respect to timesteps) is that it impedes an effective capturing of long-term dependencies [Bengio et al., 1994]. In other words, this problem limits the memory of simple RNNs, as discussed above, in effectively remembering the past.

^aOr, explode, depending on the activation function.

RNN-based models

In this section we provide more details on specific models based on RNNs, in particular LSTMs and GRU.

LSTM Long Short-Term Memory is a variation of RNN that tries to address the vanishing gradient problem. Figure 2.3 shows a high-level illustration of an LSTM network. In this high-level view, the main difference with simple RNNs (Figure 2.1) lies in the “carry” track which transfers cell states across timesteps. The carry track works as the memory of this network. An internal mechanism, called *gate*, allows the memory in LSTMs to last longer.

Figure 2.4 shows the internal architecture of an LSTM cell. Given an input word (embedding) x_t and a cell state c_t that contains the memory from the previous

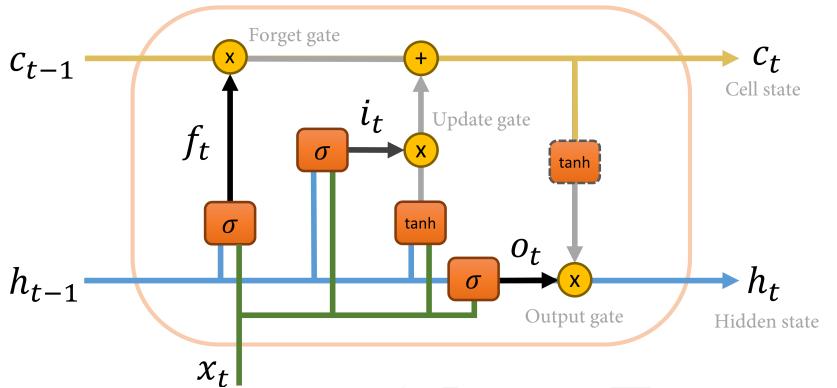


Figure 2.4: The internal structure of an LSTM cell. At timestep t , the cell “reads” an input x_t and updates the values of cell state c_t and hidden state h_t (the output of the current timestep) using three gates that control the extent to which signals can flow.

ous timesteps, the output of the current timestep h_t in the LSTM cell is computed using the following set of equations:

$$\begin{aligned}
 f_t &= \sigma(W_f x_t + U_f h_{t-1} + b_f) \\
 i_t &= \sigma(W_i x_t + U_i h_{t-1} + b_i) \\
 o_t &= \sigma(W_o x_t + U_o h_{t-1} + b_o) \\
 c_t &= f_t \circ c_{t-1} + i_t \circ \tanh(W_c x_t + U_c h_{t-1} + b_c) \\
 h_t &= o_t \circ \tanh(c_t)
 \end{aligned} \tag{2.2}$$

where \circ is the element-wise product, σ is the sigmoid function, and f_t , i_t , and o_t are the respective activation vectors for the forget, input (update), and output gates. There are three main gates in the LSTM cell that regulate the flow of information.

- The **forget** gate decides what needs to be removed from the memory. This extent, characterized by the vector f_t , is computed based on the previous state h_{t-1} and the current input x_t (line 1 in Equation 2.2). Having f_t as a vector of 1s allows all the memory to be kept, while having all 0s does the opposite. Obviously, other values of f_t allow partial retaining/forgetting of the memory.
- The **input** (update) gate controls the extent to which a new value should be placed on the memory. The activation vector for this gate is i_t which, similarly to f_t , is computed based on the previous state h_{t-1} and the current input x_t , but with different weight matrices, W_i and U_i (line 2 in Equation 2.2). The activation is multiplied by a transformed version of x_t and h_{t-1} and the resulting vector is

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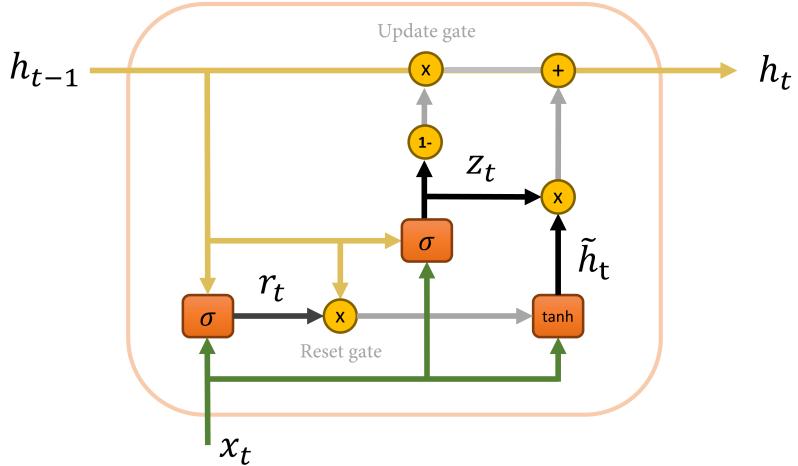


Figure 2.5: Gated Recurrent Unit (GRU) simplifies the architecture of LSTM by a few modifications, such as combining forget and input (update) gates into a single “update” gate and merging cell and hidden states.

added to the carry track c_{t-1} to form the updated cell state c_t (line 4 in Equation 2.2).

- The **output** gate controls the extent to which the “state” should be changed to compute the output of the current timestep. The output activation o_t is computed in a similar manner, by combining signals from h_{t-1} and x_t (line 3 in Equation 2.2).

The current cell state c_t is transformed through \tanh and multiplied by o_t to form the output of this timestep, i.e., h_t (last line in Equation 2.2). Similarly to other RNNs, the final cell state h_t , upon reading the last token in the sequence, can be taken as the encoded representation of the sequence. Note that the forget gate on the carry track does not involve any activation; therefore, it is theoretically possible to flow all the information through this gate and avoid the vanishing gradient problem.

GRU There are several variants of LSTM. For instance, [Gers et al. \[2003\]](#) augmented LSTMs with “peephole” connections: the activation values f_t , i_t , and o_t are computed not only based on x_t and h_{t-1} , but also based on the cell state (c_t for the latter activation and c_{t-1} for the other two activations). [Greff et al. \[2017\]](#) provide a comprehensive survey of different LSTM variants.

A famous variant is the Gated Recurrent Unit (GRU). Proposed by [\[Cho et al., 2014b\]](#), GRU combines forget and input (update) gates into a single “update” gate and

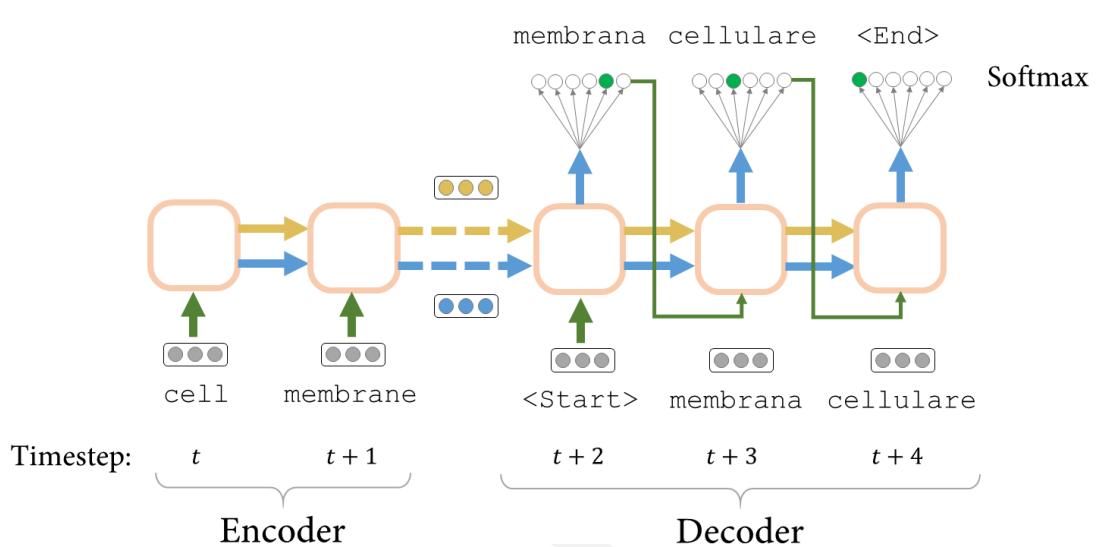


Figure 2.6: Sequence transduction based on an encoder-decoder architecture (used for translation from source to target language).

merges cell and hidden states. GRU makes use of the following equations to compute the output h_t :

$$\begin{aligned} z_t &= \sigma(W_z x_t + U_z h_{t-1} + b_z) \\ r_t &= \sigma(W_r x_t + U_r h_{t-1} + b_r) \\ \tilde{h}_t &= \tanh(W_h x_t + U_h(r_t \circ h_{t-1}) + b_h) \\ h_t &= (1 - z_t) \circ h_{t-1} + z_t \circ \tilde{h}_t \end{aligned} \tag{2.3}$$

where z_t and r_t are the respective activation vectors for the update and reset gates. Figure 2.5 shows the internal structure of a GRU cell. As can be seen from the above equations and from the figure, GRU is simpler than LSTM (it has fewer parameters). Therefore, it is less computationally expensive and faster to run.

Sequence transduction

The RNN architectures discussed so far encode a text sequence into a fixed size representation. These models are mainly suitable for cases in which a fixed-size representation for the whole input sentence is required; for instance, in sentence-level classification tasks, such as sentiment analysis. However, such RNN architectures are not suitable for tasks in which the output can vary in size. Machine Translation (MT) is a prototypical example. In this task, the translation of an input sentence can

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change in size, depending on the input and other factors, and this size is usually not known a-priori.

A branch of models called Sequence transduction or sequence to sequence (Seq2Seq) models [Sutskever et al., 2014] are suitable candidates for tasks such as MT which require input sequences to be transformed or “transduced” to the corresponding output sequences (of variable size). In other words, a Seq2Seq model converts sequences from one domain to another domain, e.g., questions to answers in Question Answering, or large pieces of texts to short texts in text summarization.

Figure 2.6 shows the high-level architecture of a typical Seq2Seq model. The model is based on the encoder-decoder structure [Sutskever et al., 2014] which is a widely-used choice for Seq2Seq models. Here, two RNN networks (usually LSTM or GRU) function as the encoder and decoder modules of this structure. The encoder transduces an input sequence (x_1, \dots, x_n) to a sequence of continuous representations $\mathbf{r} = (r_1, \dots, r_n)$. The task of the decoder is to decode the sequence \mathbf{r} into an output sequence (y_1, \dots, y_m) . The decoder is initialized with the final cell output and state of the encoder. Having a special start-of-sentence token (such as "`<Start>`") the decoder generates the first output token. The output token is the most probable word according to the softmax layer which spans over the vocabulary.

The model is *auto-regressive*. In order to generate the second output token, it consumes the previously generated symbols as additional input. In other words, at any timestep the RNN receives as its input the generated token from the previous timestep. The decoder keeps generating tokens until another special token that denotes the end of sequence (such as "`<End>`") is generated.

Attention mechanism

One issue with the encoder-decoder transduction model is that all the necessary information of the source sentence needs to be compressed into a fixed-length vector. This is especially problematic for longer sentences [Cho et al., 2014a].

Attention mechanism [Bahdanau et al., 2015] is an alignment technique to circumvent this problem. While generating output and at each timestep, the decoder performs a soft search in order to find the set of words that are most important for generating the current output token. This allows the decoder to focus on those parts of the input sequence where relevant information is concentrated. In other words, the encoder is not forced to squash all the information of the source sentence in a single fixed-size vector. Instead, it encodes the input sentence into a sequence of vectors which are later used by the decoder to generating the output sequence.

Figure 2.7 provides an illustration for the attention mechanism in an encoder-decoder sequence transduction model. While generating *cellulare*, it is natural to expect the model to look at the source word *cell*, rather than *membrane*. This is han-

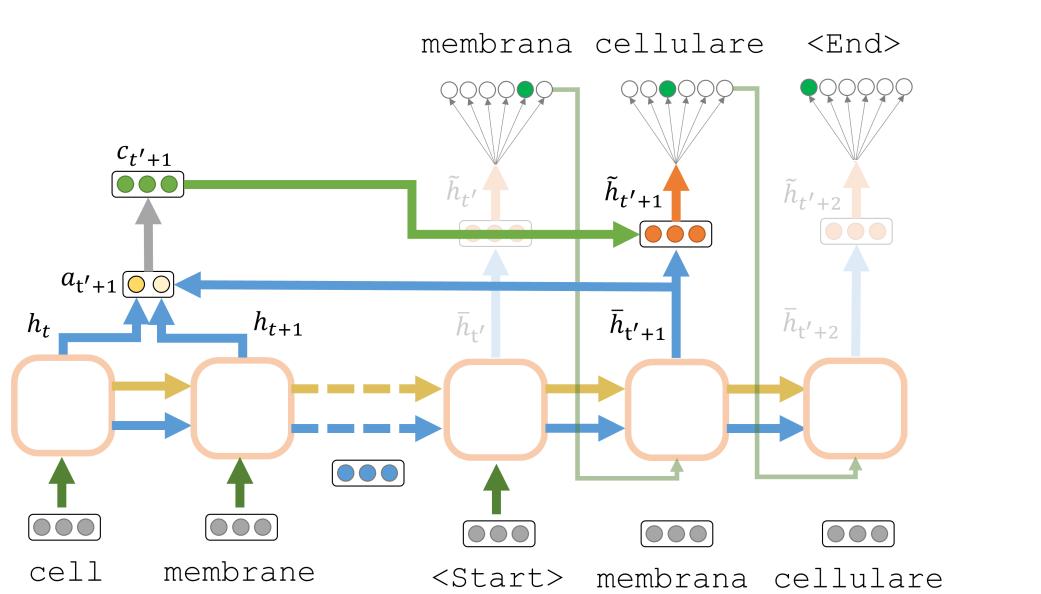


Figure 2.7: Global attention mechanism in encoder-decoder sequence transduction. During decoding, at each timestep ($t' + 1$ in the figure), the model computes an *alignment* weight vector $a_{t'+1}$ according to the current cell output $\bar{h}_{t'+1}$ and all source outputs (sequence h). The global context vector $c_{t'+1}$ is then computed as the weighted average of source outputs (weighted by $a_{t'+1}$). The attentional output $\tilde{h}_{t'+1}$ is finally computed based on $c_{t'+1}$ and $\bar{h}_{t'+1}$.

dled by the alignment vector a' , which is usually computed by combining decoder's current output $\bar{h}_{t'+1}$ and all cell outputs (sequence h) as follows:

$$a(t) = \frac{e^{score(h, \bar{h})}}{\sum_t e^{score(h, \bar{h}_t)}} \quad (2.4)$$

where $score(h, \bar{h})$ can be as simple as the dot product $h^T \bar{h}$ or other parametrized forms such as $h^T W \bar{h}$. The alignment vectors denotes those positions to which more attention needs to be paid. For the case of our example, $a_{t'+1}$ assigns more weight to *cell* than to *membrane*. The context vector c is then computed as the weighted average of h values (weighted by a).

$$c_{t'} = \sum_t a_{t'} h_t \quad (2.5)$$

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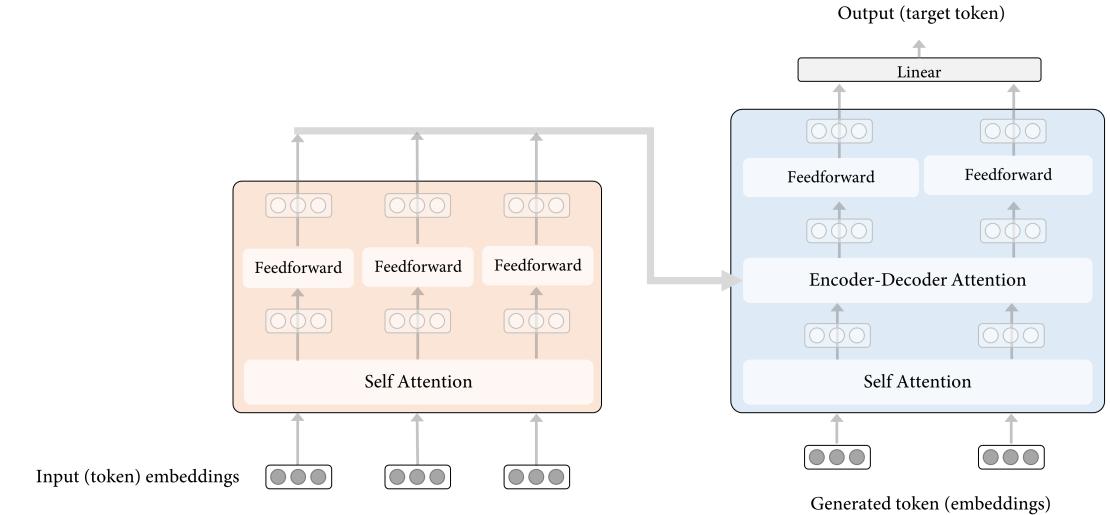


Figure 2.8: High-level architecture of the Transformer model. The sequence transduction model, which in the case of this figure translates from English to Italian, consists of stacks of encoders and decoders (more details in Chapter 6).

The context vector carries information about those source tokens which are most useful to the decoder for generating the next output token. The attentional output is finally computed using the following general formula:

$$\tilde{h}_{t'} = f(W_c[c_{t'}; \bar{h}_t]) \quad (2.6)$$

where f is the activation function of choice, e.g., \tanh . The above procedure (and the architecture in Figure 2.7) is in fact the *global context* attention mechanism proposed by Luong et al. [2015], which resembles that of [Bahdanau et al., 2015] with some simplifications.

Luong et al. [2015] also proposed a *local context* attention mechanism which aims at reducing the computational cost by constraining the context. As opposed to the global mechanism which computes the context vector based on all input words, the local mechanism focuses on a small set of input words and computes the context vector based on this set only. To this end, while generating an output token, the model first predicts a single source token (to which most attention has to be paid). Then, the context vector is computed as the weighted average of words in a window centred around the chosen source token. Luong et al. [2015] showed that the local attention mechanism not only speeds up the computation, but it also results in performance improvement in the context of neural machine translation.

2.2.3 TRANSFORMERS

Until mid 2017, RNNs were the optimal choice for encoding text sequences into fixed-size representations. However, the introduction of a model called Transformer [Vaswani et al. \[2017\]](#) revolutionized the field of machine translation, introducing a new, substantially more powerful, alternative for RNNs.

Before Transformers, the general belief was that ... without resorting to some sort of recurrence. What makes the Transformer ... interesting is that the architecture is a feed-forward model with no recurrence based on the attention mechanism only. Despite this, Transformer-based models have significantly outperformed RNNs, dominating most benchmarks for a wide range of NLP tasks that require encoding text sequences.

Figure 2.8 provides a high-level illustration of the Transformer model. Similarly to RNN-based sequence transduction models, the Transformer has an encoder-decoder architecture. However, unlike RNNs that receive input tokens sequentially, one token at a time, the Transformer model takes all the tokens in the sequence at once and in parallel. This parallel functionality makes the Transformer substantially more efficient than RNN for parallel processing. Moreover, it allows the model to “attending” to far contexts while “reading” a specific word, enabling the capture of long-distance dependencies.

Given that the Transformer architecture is tightly related with the language model-based and contextualized representations, we will discuss them with further details in Chapter 6.

2.3 KNOWLEDGE RESOURCES

Knowledge resources exist in many flavors. In this section we give an overview of knowledge resources that are mostly used for sense and concept representation learning. The nature of knowledge resources vary with respect to several factors. Knowledge resources can be broadly split into two general categories: expert-made and collaboratively-constructed. Each type has its own advantages and limitations. Expert-made resources (e.g., WordNet) feature accurate lexicographic information such as textual definitions, examples and semantic relations between concepts. On the other hand, collaboratively-constructed resources (e.g., Wikipedia or Wiktionary) provide features such as encyclopedic information, wider coverage, multilinguality and up-to-dateness.²

²In addition to these two types of resource, another recent branch is investigating the automatic construction of knowledge resources (particularly WordNet-like) from scratch [[Khodak et al., 2017](#), [Ustalov et al., 2017](#)]. However, these output resources are not yet used in practice, and they have been shown to generally lack recall [[Neale, 2018](#)].

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In the following we describe some of the most important resources in lexical semantics that are used for representation learning, namely WordNet (Section 2.3.1), Wikipedia and related efforts (Section 2.3.2), and mergers of different resources such as BabelNet and ConceptNet (Section 2.3.3).

2.3.1 WORDNET

A prominent example of expert-made resource is **WordNet** [Miller, 1995], which is one of the most widely used resources in NLP and semantic representation learning. The basic constituents of WordNet are *synsets*. A synset represents a unique concept which may be expressed through nouns, verbs, adjectives or adverbs and is composed of one or more lexicalizations (i.e., synonyms that are used to express the concept). For example, the synset of the concept defined as “the series of vertebrae forming the axis of the skeleton and protecting the spinal cord” comprises six lexicalizations: *spinal column*, *vertebral column*, *spine*, *backbone*, *back*, and *rachis*. A word can belong to multiple synsets, denoting different meanings it can take. Hence, WordNet can also be viewed as sense inventory. The sense definitions in this inventory are widely used in the literature for sense representation learning.

WordNet can alternatively be viewed as a semantic network in which nodes are synsets and edges are lexical or semantic relations (such as hypernymy or meronymy) which connect different synsets. The most recent version of WordNet version (3.1, released on 2012) covers 155,327 words and 117,979 synsets. In its way to becoming a multilingual resource, WordNet has also been extended to languages other than English through the Open Multilingual WordNet project [Bond and Foster, 2013] and related efforts.

2.3.2 WIKIPEDIA, FREEBASE, WIKIDATA AND DBPEDIA

Collaboratively-constructed knowledge resources have had substantial contribution to the research in a wide range of fields, including NLP. **Wikipedia** is one of the most prominent examples of such resources. Wikipedia is the largest multilingual encyclopedia of world and linguistic knowledge, with individual pages for millions of concepts and entities in over 250 languages. Its coverage is steadily growing, thanks to continuous updates by collaborators. For instance, the English Wikipedia alone receives approximately 750 new articles per day. Each Wikipedia article represents an unambiguous concept (e.g., *Spring (device)*) or entity (e.g., *Washington (state)*), containing a great deal of information in the form of textual information, tables, infoboxes, and various relations such as redirections, disambiguations, and categories.

A similar collaborative effort was **Freebase** [Bollacker et al., 2008]. Partly powered by Wikipedia, Freebase was a large collection of structured data, in the form of a knowledge base. As of January 2014, Freebase contained around over 40 mil-

lion entities and 2 billion relations. Freebase was finally shut down in May 2016 but its information was partially transferred to Wikidata and served in the construction of Google’s Knowledge Graph. **Wikidata** [Vrandečić, 2012] is a project operated directly by the Wikimedia Foundation with the goal of turning Wikipedia into a fully structured resource, thereby providing a common source of data that can be used by other Wikimedia projects. It is designed as a document-oriented semantic database based on *items*, each representing a topic and identified by a unique identifier. Knowledge is encoded with *statements* in the form of property-value pairs, among which definitions (descriptions) are also included. **DBpedia** [Bizer et al., 2009] is a similar effort towards structuring the content of Wikipedia. In particular, DBpedia exploits Wikipedia infoboxes, which constitutes its main source of information.

2.3.3 BABELNET AND CONCEPTNET

The types of knowledge available in the expert-based and collaboratively-constructed resources make them often complementary. This has motivated researchers to combine various lexical resources across the two categories [Niemann and Gurevych, 2011, McCrae et al., 2012, Pilehvar and Navigli, 2014]. A prominent example is **BabelNet** [Navigli and Ponzetto, 2012], which provides a merger of WordNet with a number of collaboratively-constructed resources, including Wikipedia. The structure of BabelNet is similar to that of WordNet. Synsets are the main linguistic units and are connected to other semantically related synsets, whose lexicalizations are multilingual in this case. The relations between synsets come from WordNet plus new semantic relations coming from other resources such as Wikipedia hyperlinks and Wikidata. The combination of these resources make BabelNet a large multilingual semantic network, containing 15,780,364 synsets and 277,036,611 lexico-semantic relations for 284 languages in its 4.0 release version.

ConceptNet [Speer et al., 2017] is a similar resource that combines semantic information from heterogeneous sources. In particular, ConceptNet includes relations from resources like WordNet, Wiktionary and DBpedia, as well as common-sense knowledge from crowdsourcing and games with a purpose. The main difference between ConceptNet and BabelNet lies in their main semantic units: ConceptNet models words whereas BabelNet uses WordNet-style synsets.

2.3.4 PPDB: THE PARAPHRASE DATABASE

A different kind of resource is the ParaPhrase DataBase [Ganitkevitch et al., 2013, Pavlick et al., 2015, PPDB]. PPDB is a lexical resource containing over 150 million paraphrases at different linguistic levels: lexical (single word), phrasal (multiword), and syntactic. In addition to gathering paraphrases, PPDB also has a graph structure

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where words are viewed as nodes and the edges represent mutual paraphrase connections.

CHAPTER 3

Word Embeddings

Section 1.3 briefly discussed the Vector Space Model (VSM). We saw in that section how objects can be represented using continuous vectors in an imaginary space and how distances in this space can denote the similarities between objects. However, we did not discuss how these spaces are constructed. In other words, the following question remained unanswered: how can we place hundreds of thousands of words in a space such that their positioning corresponds to their semantic properties? In this chapter, we will talk about the foundations behind constructing semantic spaces, particularly for words.

The quick answer to the above question is that semantic spaces are constructed automatically by analyzing word co-occurrences in large text corpora. But, how word co-occurrences can denote semantic similarity? The principal idea here is the **distributional hypothesis** [Firth, 1957], according to which “a word is characterized by the company it keeps.” More simply put, words that appear in similar contexts tend to have similar meanings. For instance, *Jupyter* and *Venus* tend to have similar semantics since they usually appear in similar contexts, e.g., with words such as *solar system*, *star*, *planet*, and *astronomy*. Therefore, one can collect statistics of word co-occurrences and infer semantic relationships.

Word representation learning is usually framed as an unsupervised or self-supervised procedure, in that it does not require any manual annotation of the training data. Raw texts, which are usually available at scale, can be reliably used for computing word co-occurrence statistics. Therefore, word representation techniques can automatically learn semantic spaces without needing to resort to external supervision or manual intervention. In fact, one of the winning points of VSMs, when compared to other knowledge representation approaches, is that they can be directly computed from un-annotated corpora. This is a very desirable property that has allowed VSMs to be highly flexible and extendable and therefore to dominate the field of semantic representation for many years.

However, there are several obstacles on inferring word semantics from co-occurrence statistics. We will talk about a few of these issues in this book. For instance, in addition to the celestial body meaning, *star* can refer to a well-known celebrity. Having *star* in the context of *actress* and *Jupyter* should not lead to infer-

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ring a semantic relationship between these two words. We will talk more about the ambiguity issue in Chapter 5.

In this chapter, we will specifically talk about word embeddings. Word embeddings are in fact a special type of distributed word representation that are constructed by leveraging neural networks, mainly popularised after 2013, with the introduction of Word2vec. Word embeddings are usually classified as **predictive models** because they are computed through language modeling objectives, such as predicting the next or a missing word. Before talking about predictive models in Section 3.2, we need to briefly describe the “traditional” **count-based** (Section 3.1) representations as they lay the foundation for word embeddings. We will then see the different variants and specialisation techniques for improving word embeddings, such as character embedding (Section 3.3) and knowledge-enhanced embeddings (Section 3.4), and briefly discuss cross-lingual semantic spaces (Section 3.5). This chapter concludes by common evaluation benchmarks for word embeddings (Section 3.6).

3.1 COUNT-BASED MODELS

The conventional approach for constructing VSMs was mainly based on word frequencies; therefore, the approach is usually referred to as *count-based*. Broadly speaking, the general theme in count-based models is to construct a matrix based on word frequencies. Turney and Pantel [2010] categorises count-based models based on their matrices into three general classes:

- **Term-document.** In this matrix, rows correspond to words and columns to documents. Each cell denotes the frequency of a specific word in a given document. Salton et al. [1975] first used this matrix for representing documents in order to measure the semantic similarity of pairs of documents. Two documents with similar patterns of numbers (similar columns) are deemed to be having similar topics. The term-document model is document centric; therefore, it is usually used for document retrieval, classification, or similar document-based purposes.
- **Word-context.** Unlike the term-document matrix which focuses on document representation, word-context matrix aims at representing words. Deerwester et al. [1990] first proposed using this matrix for measuring word similarity. Importantly, they extended the notion of context from documents to a more flexible definition which allowed a wide spectrum of possibilities, spanning from neighbouring words to windows of words, to grammatical dependencies or selectional preferences, to whole documents. The word-context matrix is the most widespread form of modeling and enables many applications and tasks,

such as word similarity measurement, word sense disambiguation, semantic role labeling, and query expansion.

- **Pair-pattern.** In this matrix, rows correspond to pairs of words and columns are the patterns in which the two have occurred. [Lin and Pantel \[2001\]](#) used this to find similarity of patterns, e.g. “X is the author of Y” and “Y is written by X”. The matrix is suitable for measuring relational similarity: the similarity of semantic relations between pairs of words, e.g., “linux:grep” and “windows:findstr”. [Lin and Pantel \[2001\]](#) first proposed *extended distributional hypothesis*: patterns that co-occur with similar pairs (contexts) tend to have similar meanings.

The earliest VSM applied in NLP considered a document as a vector whose dimensions were the whole vocabulary [\[Salton et al., 1975\]](#). Weights of individual dimensions were initially computed based on word frequencies within the document. Different weight computation metrics have been explored, but mainly based on frequencies or normalized frequencies [\[Salton and McGill, 1983\]](#). This methodology has been successfully refined and applied to various NLP applications such as information retrieval [\[Lee et al., 1997\]](#), text classification [\[Soucy and Mineau, 2005\]](#), or sentiment analysis [\[Turney, 2002\]](#), to name a few. In this book we will focus on newer forms of representation (i.e. embeddings), and we would recommend the extensive survey of [\[Turney and Pantel \[2010\]\]](#), which provides a comprehensive overview of earlier VSM and their applications, for more detailed information.

The document-based VSM has been also extended to other lexical items like words. In this case a word is generally represented as a point in a vector space. A word-based vector has been traditionally constructed based on the normalized frequencies of the co-occurring words in a corpus [\[Lund and Burgess, 1996\]](#), by following the initial theories of [Harris \[1954\]](#). The main idea behind word VSM is that words that share similar context should be close in the vector space (therefore, have similar semantics). Figure 1.3 shows an example of a word VSM where this underlying proximity axiom is clearly highlighted.

3.1.1 POINTWISE MUTUAL INFORMATION

Raw frequencies does not provide a reliable measure of association. A “stop word” such as “the” can frequently co-occur with a given word, but this co-occurrence does not necessarily correspond to a semantic relationship, since it is not discriminative. It is more desirable to have a measure that can incorporate the informativeness of a co-occurrence. Positive Pointwise Mutual Information (PPMI) is such a measure [\[Church and Hanks, 1990\]](#). PMI normalizes the importance of the co-occurrence of two words by their individual frequencies.

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$$PMI(w_1, w_2) = \log_2 \frac{P(w_1, w_2)}{P(w_1)P(w_2)} \quad (3.1)$$

where $P(x)$ is the probability of word x which can be directly computed based on its frequency. PMI checks if w_1 and w_2 co-occur more than they occur independently. A stop word has a high P value, resulting in a reduced overall PMI value. PMI values can range from $-\infty$ to $+\infty$. Negative values indicate a co-occurrence which is less likely to happen than by chance. Given that these associations are computed based on highly sparse data and that they are not easily interpretable (it is hard to define what it means for two words to be very “unrelated”), we usually ignore negative values and replace them with 0, hence Positive PMI (PPMI).

3.1.2 DIMENSIONALITY REDUCTION

The word-context modeling is the most widespread way to compute count-based word representations. Usually, words that co-occur with the target word are taken as its *context*. Therefore, the number of columns¹ in this matrix is equal to the number of words in the vocabulary (i.e., unique words in a corpus). This number can easily reach hundreds of thousands or even millions, depending on the underlying corpus. This can potentially be a limiting factor, given that large vectors are less favorable due to storage space and computational reasons. To circumvent this limitation, a dimensionality reduction procedure is usually applied to VSM representations.

Dimensionality reduction can be obtained by simply dropping those *contexts* (i.e., columns) which are less informative or important (for instance, frequent function words). This can be done using feature selection techniques. But, we can also reduce dimension by merging or combining multiple columns into fewer new columns. The latter case is the basis for Singular Value Decomposition (SVD), which is a common approach for dimensionality reduction of VSMs.

SVD consists of factorizing a given $m \times n$ matrix into three component matrices $U\Sigma V^*$, where Σ is an $m \times n$ diagonal matrix whose diagonal entries are called “singular values”. One can reconstruct the original matrix based on these three. But, interestingly, it is also possible to reconstruct an approximation of the original matrix (with smaller dimensionality). To this end, one can pick only the set of k largest singular values (discarding the rest) and use that to reconstruct an $m \times k$ approximation of the original matrix. With SVD, word representations are now reduced in size from n dimensions to k (where $n \ll k$). Reducing dimensionality can bring additional advantages, such as eliminating noise. Note that the new k dimensions are not more interpretable.

¹The number of columns and rows in the word-context should be equal if we are interested in representing all words

One of the key features of neural networks is their ability to learn dense representations. In what follows, we will see some techniques that leverage neural networks to directly learn low-dimensional word representations, without needing to resort to the additional dimensionality reduction step.

3.2 PREDICTIVE MODELS

Learning low-dimensional vectors from text corpora can alternatively be achieved by leveraging neural networks. The representations that are generated using neural networks are commonly referred to as *embedding*, particularly due to their property of being dense and low dimensional. Neural networks were suitable candidates for this purpose due to their efficiency and speed in processing large amounts of texts and for their ability in learning dense representations [Bengio et al., 2003, Collobert and Weston, 2008, Turian et al., 2010, Collobert et al., 2011]. However, their success was limited due to hardware and software limitations of deep learning. In the last decade, together with the growth of deep learning, neural network based representations (embeddings) have almost fully replaced the conventional count-based models and dominated the field. Given that neural word embeddings are usually trained with some sort of language modeling objective, such as predict a missing word in a context, they are also referred to as predictive models. Word embeddings were popularized by Word2vec [Mikolov et al., 2013a].

Word2Vec. Word2vec [Mikolov et al., 2013d] is based on a simple but efficient feedforward neural architecture which is trained with language modeling objective. Two different but related Word2vec models were proposed: Continuous Bag-Of-Words (CBOW) and Skip-gram. The CBOW model aims at predicting the current word using its surrounding context, minimizing the following loss function:

$$E = -\log(p(\vec{w}_t | \vec{W}_t)) \quad (3.2)$$

where w_t is the target word and $W_t = w_{t-n}, \dots, w_t, \dots, w_{t+n}$ represents the sequence of words in context. The Skip-gram model is similar to the CBOW model but in this case the goal is to predict the words in the surrounding context given the target word, rather than predicting the target word itself.

Figure 3.1 shows a simplification of the general architecture of the CBOW and Skip-gram models of Word2vec. The architecture consists of input, hidden and output layers. The input layer has the size of the word vocabulary and encodes the context as a combination of one-hot vector representations of surrounding words of a given target word. The output layer has the same size as the input layer and contains a one-hot vector of the target word during the training

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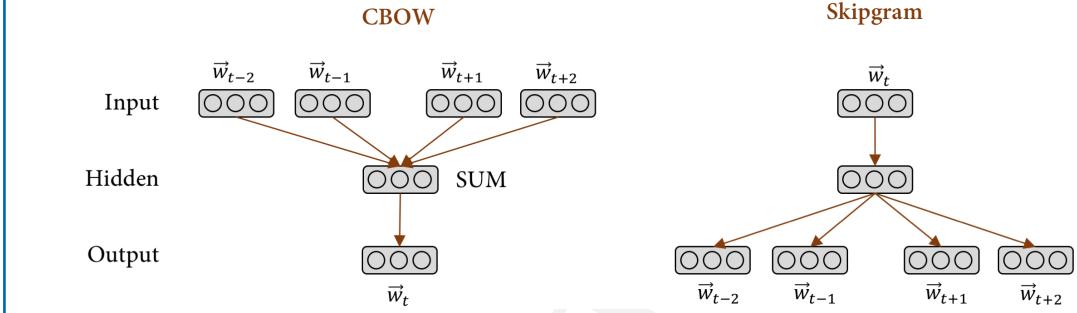


Figure 3.1: Learning architecture of the CBOW and Skipgram models of Word2vec [Mikolov et al., 2013a].

phase. Interestingly, Levy and Goldberg [2014b] proved that Skip-gram can be in fact viewed as an implicit factorization of a Pointwise Mutual Information (PMI) co-occurrence matrix (Section 3.1.1).

Another prominent word embedding architecture is GloVe [Pennington et al., 2014], which tries to perform the meaning embedding procedure of Word2vec in an explicit manner. The main idea behind GloVe is that the ratio of co-occurrence probabilities of two words, w_i and w_j , with a third probe word w_k , i.e., $P(w_i, w_k)/P(w_j, w_k)$, is more indicative of their semantic association than a direct co-occurrence probability, i.e., $P(w_i, w_j)$. To achieve this, they propose an optimization problem which aims at fulfilling the following objective:

$$w_i^T w_k + b_i + b_k = \log(X_{ik}) \quad (3.3)$$

where b_i and b_k are bias terms for word w_i and probe word w_k and X_{ik} is the number of times w_i co-occurs with w_k . Fulfilling this objective minimizes the difference between the dot product of w_i and w_k and the logarithm of their number of co-occurrences. In other words, the optimization results in the construction of vectors w_i and w_k whose dot product gives a good estimate of their transformed co-occurrence counts.

Note that GloVe does not make use of neural networks. However, Levy et al. [2015] consider it as a predictive model, mainly since GloVe was proposed with the new wave of neural word embeddings and was different from conventional count-based models in that it uses Stochastic Gradient Descent to optimize a non-convex objective, whereas SVD guarantees an optimal decomposition (according to its objective).

In recent years more complex approaches that attempt to improve the quality of word embeddings have been proposed, including models exploiting depen-

dency parse-trees [Levy and Goldberg, 2014a] or symmetric patterns [Schwartz et al., 2015], leveraging subword units [Wieting et al., 2016, Bojanowski et al., 2017], representing words as probability distributions [Vilnis and McCallum, 2015, Athiwaratkun and Wilson, 2017, Athiwaratkun et al., 2018], learning word embeddings in multilingual vector spaces [Conneau et al., 2018b, Artetxe et al., 2018b], or exploiting knowledge resources (more details about this type in Section 3.4).

3.3 CHARACTER EMBEDDING

Even when the vocabulary of a word embedding space is large, we can encounter situations where a word is out of vocabulary (OOV). The default solution for such cases is to assign a random embedding to the OOV word. This is indeed not a good solution, especially if it is an importance word that plays a central role in our understanding of the context and in decision making.

There is a literature on unseen word representation. Given that many of the OOV words can be morphological variations of existing words in the vocabulary, a large body of work has focused on this type of unseen word representation [Lazari-dou et al., 2013, Botha and Blunsom, 2014, Soricut and Och, 2015]. To this end, usually a morphological segmenter is used to break inflected words into their components and to compute representations by extending the semantics of an unseen word’s morphological variations. For instance, an unseen word like *memoryless* can be broken into *memory* and *less*. An embedding can be induced for the unseen word based on the embeddings of its individual components *memory* and *less* which are more frequent and probably seen during the training.

Alternatively, the word can be broken into constituent subwords, i.e., group of characters that are not necessarily semantically meaningful. FastText [Bojanowski et al., 2017] is a prominent example for such an approach. In addition to words appearing in the training corpus, the model learns embeddings for n-grams of these words. Then, in the case of an unseen word, the corresponding embedding is induced by averaging the vector representations of its constituent character n-grams. This provides a quick solution for OOV embedding, but not an optimal one given that two words can have similar n-gram constituents but be dissimilar in terms of semantics.

Another approach for unseen word representation is to exploit knowledge from external lexical resources, such as WordNet, in order to induce an embedding for the unseen word (with the assumption that the word is covered in WordNet). For instance, Pilehvar and Collier [2017a] extract from WordNet a set of semantically similar words to the OOV word and combine their embeddings to form an embedding for the OOV word. Bahdanau et al. [2017] take a similar approach and leverage the definition of the missing word (again taken from WordNet) to induce its repre-

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sentation. These techniques make the assumption that the OOV word is covered in the underlying lexical resource, which might not be necessarily true.

It is also possible to change the architecture of the NLP system so that it receives sequences of characters as its input, instead of the usual sequence of word tokens. Such character-based models are usually coupled with LSTM networks, with the hope to capture character order and also sequential patterns. Such character-based models have been successfully tested in different NLP tasks, including language modeling [Sutskever et al., 2011, Graves, 2013], part-of-speech tagging [Dos Santos and Zadrozny, 2014, Ling et al., 2015], syntactic parsing [Ballesteros et al., 2015], and machine translation [Lee et al., 2017, Kalchbrenner et al., 2016].

3.4 KNOWLEDGE-ENHANCED WORD EMBEDDINGS

As explained throughout this chapter, word vector representations (e.g., word embeddings) are mainly constructed by exploiting information from text corpora only. However, there is also a line of research which tries to combine the information available in text corpora with the knowledge encoded in lexical resources. This knowledge can be leveraged to include additional information not available in text corpora in order to improve the semantic coherence or coverage of existing word vector representations. Moreover, knowledge-enhanced word representation techniques are closely related to knowledge-based sense representation learning (see next section), as various models make use of similar techniques interchangeably.

The earlier attempts to improve word embeddings using lexical resources modified the objective function of a neural language model for learning word embeddings (e.g., Skip-gram of Word2vec) in order to integrate relations from lexical resources into the learning process [Xu et al., 2014, Yu and Dredze, 2014]. A more recent class of techniques, usually referred to as *retrofitting* [Faruqui et al., 2015], attempts at improving pre-trained word embeddings with a post-processing step. Given any pre-trained word embeddings, the main idea of retrofitting is to move closer words which are connected via a relationship in a given semantic network². The main objective function to minimize in the retrofitting model is the following:

$$\sum_{i=1}^{|V|} \left(\alpha_i \|\vec{w}_i - \hat{\vec{w}}_i\| + \sum_{(w_i, w_j) \in N} \beta_{i,j} \|\vec{w}_i - \vec{w}_j\| \right) \quad (3.4)$$

where $|V|$ represents the size of the vocabulary, N is the input semantic network represented as a set of word pairs, \vec{w}_i and \vec{w}_j correspond to word embeddings in the pre-trained model, α_i and $\beta_{i,j}$ are adjustable control values, and $\hat{\vec{w}}_i$ represents the output word embedding.

²FrameNet [Baker et al., 1998], WordNet and PPDB [Ganitkevitch et al., 2013] are used in their experiments.

Building upon retrofitting, Speer and Lowry-Duda [2017] exploited the multilingual relational information of ConceptNet for constructing embeddings on a multilingual space, and Lengerich et al. [2017] generalized retrofitting methods by explicitly modeling pairwise relations. Other similar approaches are those by Pilehvar and Collier [2017b] and Goikoetxea et al. [2015], which analyze the structure of semantic networks via Personalized Page Rank [Haveliwala, 2002] for extending the coverage and quality of pre-trained word embeddings, respectively. Finally, Bollegala et al. [2016] modified the loss function of a given word embedding model to learn vector representations by simultaneously exploiting cues from both co-occurrences and semantic networks.

Recently, a new branch that focuses on specializing word embeddings for specific applications has emerged. For instance, Kiela et al. [2015] investigated two variants of retrofitting to specialize word embeddings for similarity or relatedness, and Mrksic et al. [2017] specialized word embeddings for semantic similarity and dialogue state tracking by exploiting a number of monolingual and cross-lingual linguistic constraints (e.g., synonymy and antonymy) from resources such as PPDB and BabelNet.

In fact, as shown in this last work, knowledge resources also play an important role in the construction of multilingual vector spaces. The use of external resources avoids the need of compiling a large parallel corpora, which has been traditionally been the main source for learning cross-lingual word embeddings in the literature [Upadhyay et al., 2016, Ruder et al., 2017]. These alternative models for learning cross-lingual embeddings exploit knowledge from lexical resources such as WordNet or BabelNet [Mrksic et al., 2017, Goikoetxea et al., 2018], bilingual dictionaries [Mikolov et al., 2013b, Ammar et al., 2016, Artetxe et al., 2016, Doval et al., 2018] or comparable corpora extracted from Wikipedia [Vulić and Moens, 2015]. In the following section we provide more details on these approaches and cross-lingual word embedding learning in general.

3.5 CROSS-LINGUAL WORD EMBEDDINGS

Cross-lingual word embeddings are an extended notion of word embeddings where words from two or more languages are represented in the same shared low-dimensional vector space. Intuitively, these spaces preserve similar properties than standard monolingual word embeddings.

For a more comprehensive overview of cross-lingual word embeddings we recommend the book from this editorial of Søgaard et al. [2019]. In the following we split the different types of word embedding by their source of supervision: sentence-level (Section 3.5.1), document-level (Section 3.5.2), word-level (Section 3.5.3) and unsupervised (Section 3.5.4).

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3.5.1 SENTENCE-LEVEL SUPERVISION

The kind of supervision for these models lie generally on parallel corpora, of the same type used for Machine Translation, e.g., Europarl [Koehn, 2005]. This is extensive for many high-resource language pairs, but sometimes hard to obtain it, at least publicly, for other less-resources languages. Given their similarity with Machine Translation, the methods to learn cross-lingual with this kind of supervision are often interchangeable. Examples of cross-lingual embedding learned from sentence alignments are Hermann and Blunsom [2014] or Lauly et al. [2014] which use compositional functions and autoencoders, respectively.

3.5.2 DOCUMENT-LEVEL SUPERVISION

This kind of supervision involves full comparable documents (not necessarily translations) which versed about the same domain. The most prominent example of this kind of supervision is Wikipedia, where documents in different languages explain the same concept or domain. This supervision is arguably easier to obtain than sentence translations and, in the worst case, fully translated documents could also be used for supervision. For instance, Vulic and Moens [2016] make use of Wikipedia pages of the same concept or entity in different languages. These different Wikipedia versions are not exact translations but rather deal with the same topic.

3.5.3 WORD-LEVEL SUPERVISION

To learn cross-lingual embeddings with word-level supervision, only a bilingual dictionary is necessary. This branch has been quite attractive for some time due to this cheap supervision, as bilingual dictionaries are easily available for hundreds of language pairs.

These methods are in the main based on linear alignments that map words from the input languages to their translations in the target language. A prominent example of such method is the proposal of Mikolov et al. [2013b]. Specifically, they proposed to learn a matrix \mathbf{W} which minimizes the following objective:

$$\sum_{i=1}^n \|\mathbf{x}_i \mathbf{W} - \mathbf{z}_i\|^2 \quad (3.5)$$

where we write \mathbf{x}_i for the vector representation of some word x_i in the source language and \mathbf{z}_i is the vector representation of the translation z_i of w_i in the target language. This optimization problem corresponds to a standard least-squares regression problem, whose exact solution can be efficiently computed. Note that this approach relies on a bilingual dictionary containing the training pairs $(x_1, z_1), \dots, (x_n, z_n)$. However, once the matrix \mathbf{W} has been learned, for any word w in the source language,

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we can use xW as a prediction of the vector representation of the translation of w . In particular, to predict which word in the target language is the most likely translation of the word w from the source language, we can then simply take the word z whose vector z is closest to the prediction xW .

The restriction to linear mappings might intuitively seem overly strict. However, it was found that higher-quality alignments can be found by being even more restrictive. In particular, [Xing et al. \[2015\]](#) suggested to normalize the word vectors in the monolingual spaces, and restrict the matrix W to an orthogonal matrix (i.e., imposing the constraint that $WW^T = 1$). Under this restriction, the optimization problem (3.5) is known as the orthogonal Procrustes problem, whose exact solution can still be computed efficiently. Another approach was taken by [Faruqui and Dyer \[2014\]](#), who proposed to learn linear transformations W_s and W_t , which respectively map vectors from the source and target language word embeddings onto a shared vector space. They used Canonical Correlation Analysis to find the transformations W_s and W_t which minimize the dimension-wise covariance between XW_s and ZW_t , where X is a matrix whose rows are x_1, \dots, x_n and similarly Z is a matrix whose rows are z_1, \dots, z_n . Note that while the aim of [Xing et al. \[2015\]](#) is to avoid making changes to the cosine similarities between word vectors from the same language, [Faruqui and Dyer \[2014\]](#) specifically want to take into account information from the other language with the aim of improving the monolingual embeddings themselves. On top of this, [Artetxe et al. \[2018a\]](#) proposed a multi-step framework in which they experiment with several pre-processing and post-processing strategies. These include whitening (which involves applying a linear transformation to the word vectors such that their covariance matrix is the identity matrix), re-weighting each coordinate according to its cross-correlation (which means that the relative importance of those coordinates with the strongest agreement between both languages is increased), de-whitening (i.e., inverting the whitening step to restore the original covariances), and dimensionality reduction step, which is seen as an extreme form of re-weighting (i.e., those coordinates with the least agreement across both languages are simply dropped). They also consider the possibility of using orthogonal mappings of both embedding spaces into a shared space, rather than mapping one embedding space onto the other, where the objective is based on maximizing cross-covariance. Other approaches that have been proposed for aligning monolingual word embedding spaces include models which replace (3.5) with a max-margin objective [Lazaridou et al. \[2015\]](#) and models which rely on neural networks to learn non-linear transformations [Lu et al. \[2015\]](#).

Postprocessing. By restricting transformations to orthogonal linear mappings, these methods rely on the assumption that the monolingual embeddings spaces

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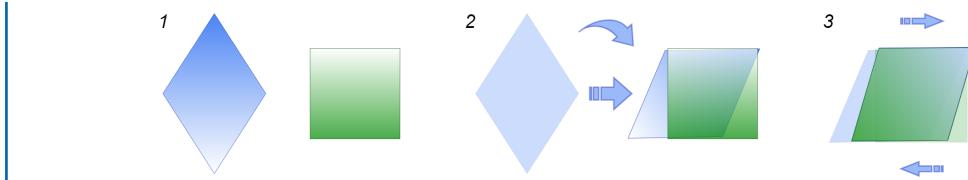


Figure 3.2: Two-stage procedure for mapping two monolingual word embedding spaces together [Doval et al., 2018].

are approximately isomorphic [Barone, 2016, Doval et al., 2019]. However, it has been argued that this assumption is overly restrictive, as the isomorphism assumption is not always satisfied [Søgaard et al., 2018]. For this reason, it has been proposed to go beyond orthogonal transformations by modifying the internal structure of the monolingual spaces, either by giving more weight to highly correlated embedding components, as is the case for unsupervised variants [Artetxe et al., 2018a], or by complementing the orthogonal transformation with other forms of post-processing. As an example of this latter strategy, Doval et al. [2018] fine-tune the initial alignment by learning an unconstrained linear transformation which aims to map each word vector onto the average of that vector and the corresponding word vector from the other language.

Figure 3.2 shows a common pipeline including an orthogonal transformation and a final post-processing to further approach the resulting embedding spaces.

3.5.4 UNSUPERVISED

This branch of cross-lingual embeddings deals with those approaches that do not need for any kind of external supervision. Generally, unsupervised models learn language-specific embeddings from monolingual corpora and then learn a bilingual dictionary based on the distribution of these embeddings. This bilingual dictionary can also be learned leveraging using distant supervision techniques, such as constructing dictionaries from identical tokens [Smith et al., 2017] or numerals [Artetxe et al., 2017] or exploiting structural similarities of the monolingual vector spaces.

From this branch techniques to learn a bilingual dictionary automatically from the monolingual embeddings can be split into two main categories: adversarial and distributional. One of the prominent works exploiting adversarial techniques is Conneau et al. [2018b]. This approach relies on adversarial training [Goodfellow et al., 2014], similar as in earlier models [Barone, 2016, Zhang et al., 2017b] but using a simpler formulation, based on the model in (3.5) with the orthogonality constraint on

\mathbf{W} . The main intuition is to choose \mathbf{W} such that it is difficult for a classifier to distinguish between word vectors \mathbf{z} sampled from the target word embedding and vectors $\mathbf{x}\mathbf{W}$, with \mathbf{x} sampled from the source word embedding. There have been other approaches to create this initial bilingual dictionary without supervision via adversarial training [Zhang et al., 2017a, Hoshen and Wolf, 2018, Xu et al., 2018] or stochastic processes [Alvarez-Melis and Jaakkola, 2018]. These approaches have attempted to improve the robustness of the initial adversarial alignment, which have been shown not robust in different settings and especially on far languages [Søgaard et al., 2018]. As for non-adversarial techniques, Artetxe et al. [2018b] obtain the initial seed dictionary automatically by leveraging the similarity histogram distribution of words in the source and target languages. The underlying idea is that word translation in different languages will have similar distributions with respect to their distance to the other words in the vocabulary.

Finally, once this bilingual dictionary is constructed, cross-lingual embeddings are learned by making use of the word-level techniques presented in Section 3.5.3.

3.6 EVALUATION

In this section we present the most common evaluation benchmarks for assessing the quality of word representations. Depending on their nature, evaluation procedures are generally divided into intrinsic (Section 3.6.1) and extrinsic (Section 3.6.2).

3.6.1 INTRINSIC EVALUATION

Intrinsic evaluation refers to a class of benchmarks that provide a generic evaluation of the quality and coherence of a vector space, independently from their performance in downstream applications. Different properties can be intrinsically tested, with semantic similarity being traditionally viewed as the most straightforward feature to evaluate meaning representations. In particular, the semantic similarity of small lexical units such as words, in which compositionality is not required, has received the most attention. Word similarity datasets exist in many flavors.

It is also worth distinguishing the notions of similarity and relatedness. Two words are deemed to be semantically *similar* if they share many properties (e.g., “bike” and “motorcycle”, “lime” and “lemon”) whereas they are semantically *related* as long as they have any semantic relationship, such as meronymy (e.g., “wheel” and “bike”) or antonymy (“sunset” and “sunrise”). While words that are semantically similar can be technically substituted with each other in a context, related words are enough to co-occur in the same context (e.g., within a document) without the need for substitutability.

The original WordSim-353 [Finkelstein et al., 2002] is a dataset that conflates these two notions. Agirre et al. [2009] divided the pairs in the dataset into two new

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subsets with the aim of distinguishing similarity and relatedness. Genuine similarity datasets include RG-65 [Rubenstein and Goodenough, 1965] and C-30 [Miller and Charles, 1991], which only contains 65 and 30 word pairs, respectively, or SimLex-999 [Hill et al., 2015], consisting of 999 word pairs. For a more comprehensive survey on semantic relatedness evaluation procedures, the reader could refer to Taieb et al. [2019].

As long as intrinsic evaluation benchmarks are concerned for languages other than English, very few word similarity datasets exist. Equivalents of the originally-English RG-65 and WordSim-353 datasets are constructed via translating these datasets either by experts [Gurevych, 2005, Joubarne and Inkpen, 2011, Granada et al., 2014, Camacho-Collados et al., 2015], or by means of crowdsourcing [Leviant and Reichart, 2015]. Similarly, for the cross-lingual representations, most intrinsic benchmarks are constructed based on standard English word similarity datasets: MC-30 [Miller and Charles, 1991] and WordSim-353 [Hassan and Mihalcea, 2011], and RG-65 [Camacho-Collados et al., 2015]. The procedure is based on aligning pairs across different versions of the same dataset in different languages. However, these datasets are either too small to allow a reliable comparison of models and to draw concrete conclusions, or they inherit the conflated similarity scale of the WordSim-353 dataset. SemEval-2017 Task 2 [Camacho-Collados et al., 2017] was aimed at addressing these issues by introducing several relatively large multilingual and cross-lingual datasets annotated by experts according to a refined scale.

In addition to word similarity, measuring relational similarity has been used as a means of evaluating word representations, especially word embeddings. One of the popular evaluation benchmark for the purpose was constructed by Mikolov et al. [2013c]. Given a pair (e.g., *brother* and *sister*) and a third word (e.g., *grandson*) the goal is to find the pairing word for the third word that matches the semantic relationship between the words in the first pair (e.g., *granddaughter*). Other intrinsic evaluation procedures include synonymy selection [Landauer and Dumais, 1997, Turney, 2001, Jarmasz and Szpakowicz, 2003, Reisinger and Mooney, 2010], outlier detection [Camacho-Collados and Navigli, 2016, Blair et al., 2016, Stanovsky and Hopkins, 2018], and selectional preferences and concept categorization [Baroni et al., 2014]. For more information, Bakarov [2018] provides a more comprehensive overview of intrinsic evaluation benchmarks.

Problems with intrinsic evaluations

Several problems have been pointed out by various researchers on the intrinsic evaluations of word representations. An important limitation is that word similarity benchmarks often consider only the *attributional* similarity of words, i.e., the extent of correspondence between the properties of two words. However, different tasks in NLP

deal with different notions of similarity, which might not necessarily match attributional similarity. For instance, word embeddings to be used for a POS tagging model do not need to encode fine-grained semantic distinctions, e.g., having identical representations for *cat* and *tiger* and even *giraffe* might not be an issue. However, for a Question Answering system, fine-grained distinctions such as that between *south* and *north* might be critical: there is a huge difference between answering “around sunset” and “around sunrise” when asked “when is best to visit the museum?”. The SimLex-999 dataset is designed with the intention to highlight this notion of similarity: For instance the score assigned to the pair “sunset”:“sunrise” is lower than that for “bed”:“bedroom” and “paper”:“wood”.

Given the variability in the notion of similarity, one might expect word embeddings to behave differently in various NLP tasks. In fact, it is shown by various researchers that intrinsic evaluation protocols do not always correlate with downstream performance. [Tsvetkov et al. \[2015\]](#) showed that performance on standard word similarity benchmarks has a low correlation with results on tasks such as sentiment analysis, metaphor detection and text classification, whereas [Chiu et al. \[2016\]](#) found that, strikingly, there is a negative correlation between word similarity performance and results on Named Entity Recognition.

[Tsvetkov et al. \[2015\]](#) proposed an alternative intrinsic evaluation, called QVEC, which is based on aligning a word embedding matrix to the matrix of features extracted from manually crafted lexical resources. Specifically, they use SemCor [[Miller et al., 1993](#)], a large sense-annotated corpus, to construct a custom word-context matrix where rows are words and columns are WordNet supersenses (which are 41 in total). The columns in this matrix are aligned with the columns in the corresponding word representation matrix (which is to be evaluated) by maximizing correlation. The central assumption is that dimensions in the latter matrix correspond to linguistic properties in the former matrix. The degree of “semantic content” is then computed as the total correlation among these two matrices. It was shown that QVEC can produce better estimates of downstream performance when compared to standard word similarity evaluations.

Another important problem with intrinsic evaluation is due to hubness. A hub in the semantic space is a word that has high cosine similarity with a large number of other words [[Lazaridou et al., 2015](#)]. Pairs of words with similar frequency tend to be closer in the semantic space, thus showing higher word similarity than they should [[Schnabel et al., 2015](#)].

Ignoring the polysemous nature of words is another issue with most existing intrinsic evaluation benchmarks. Most word similarity benchmarks do not check for the ability of embedding models in capturing different meanings of a word. For an embedding model to succeed on these benchmarks, it is often enough to encode

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the most frequent meaning of a word. In chapter 5 we will talk in detail about the desired property of word embeddings in capturing various meanings. For a more detailed review of problems associated with word embeddings, the reader might refer to [Faruqui et al. \[2016\]](#).

3.6.2 EXTRINSIC EVALUATION

Extrinsic evaluation procedures aim at assessing the quality of vector representations when used as input features to a machine learning model in a downstream NLP task. In addition to intrinsic evaluation procedures, extrinsic evaluation is necessary to understand the effectiveness of word representation techniques in real-world applications. This is especially relevant given the problems listed with currently practised intrinsic evaluations.

In fact, any NLP application that deals with lexical semantics can be used for extrinsic evaluation of word representation. In their seminal work on the use of neural networks for NLP, [Collobert et al. \[2011\]](#) used a wide range of tasks including part of speech tagging, chunking, named entity recognition, and semantic role labeling. Though the goal in this work was not exactly the explicit evaluation of word embeddings, one can use the framework for comparing various word embeddings by introducing them to the model as input features while fixing the network configuration. Text classification tasks such as sentiment analysis, metaphor detection, and topic categorization have also been used in the context of word embedding evaluation [[Schnabel et al., 2015](#), [Tsvetkov et al., 2015](#)].

Extrinsic evaluations are reflecting the performance of a word embedding in a downstream scenario, but, similarly to intrinsic evaluations, they are prone to limitations which make them insufficient as a sole basis for evaluating word embeddings. The first limitation is shared to some extent between intrinsic and extrinsic evaluations and comes from the fact that different NLP tasks might highly differ in their nature. In fact, word embedding performance does not necessarily correlate across tasks [[Schnabel et al., 2015](#)]. This makes it impossible to prescribe a single best-performing solution for all NLP tasks. For instance, word embeddings suitable for part of speech tagging might perform no better than random embeddings on sentiment analysis. Conclusions drawn from such evaluations should be limited to the specific task or the group of similar tasks and cannot be generalised to other tasks with different nature.

The second limitation arises from the fact that it is more difficult to control all the factors in extrinsic evaluation frameworks. In a typical NLP system, there are many parameters that play role in the final performance; sometimes even small changes in the configuration might drastically change the results. This makes it more difficult to draw general reliable conclusions from extrinsic evaluations. An embed-

ding model performing well in a specific system configuration, for instance in sentiment analysis, might not necessarily perform well in other sentiment analysis systems or even different configurations of the same model. Therefore, one should be very careful with the use of evaluation benchmarks, and more importantly, with the conclusions they make. It is always recommended to employ a mixture of intrinsic and extrinsic evaluations, and on a diverse range of datasets and tasks.

CHAPTER 4

Graph Embeddings

Graphs are ubiquitous data structures. They are often the preferable choice for representing various type of data, including social networks, word co-occurrence and semantic networks, citation networks, telecommunication networks, molecular graph structures and biological networks. Therefore, analyzing them can play a central role in various real-world scenarios, such as drug design, friendship recommendation in social networks, semantic modeling in language, and communication pattern extraction.

For instance, consider Zachary's famous Karate Club social network [Zachary, 1977] in Figure 4.1 (left). The network has 34 members which are shown as nodes in the graph. Edges in this graph denote if any pair of members had interactions outside of the club. Representing this social network as a graph facilitates its interpretation and analysis. With the first look, one can quickly have an idea on the rough number of friends each member in this network has by average, identify communities in the network, or find those members (nodes) that have so many friends and are central in a community or bridge different communities.

The primary challenge in graph embedding is to find a way to represent the data stored in a graph in a machine-interpretable or mathematical format which would allow the application of machine learning models. In other words, the high-dimensional, non-Euclidean graph structure needs to be encoded into a numerical or feature-based form.

We view the task of graph embedding from two different perspectives:

1. **Node embedding**, in which the aim is to embed the nodes of a graph into a continuous semantic space with the objective of preserving relative “distances” (to be discussed in the following section).
2. **Relation embedding**, in which the edges in the graph, i.e., the relationships between nodes, are the target of attention for embedding. We further categorise relation embedding techniques into **knowledge-based** relation embedding models (Section 4.2) and **unsupervised** models (Section 4.3).

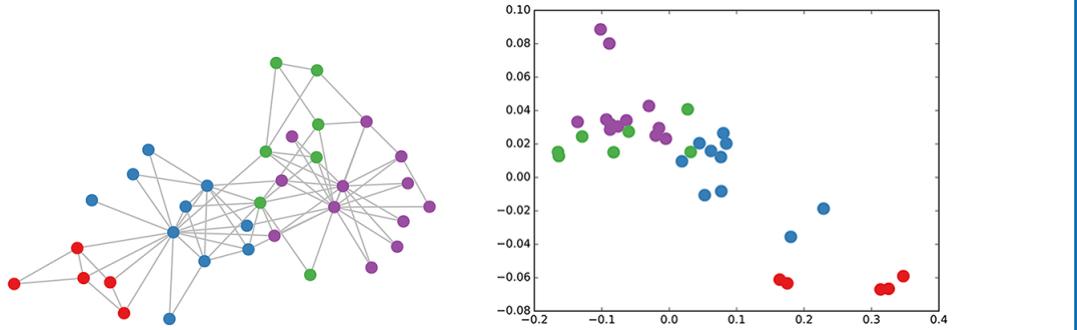


Figure 4.1: Zachary Karate Club graph (left) and the corresponding embedding space computed by Graph Convolutional Networks (GCN). Communities, as detected by modularity-based clustering [Brandes et al., 2008], are shown by different colors. Graph embedding tries to encode properties of graph nodes (such as neighbourhood) in a continuous multidimensional space (in this case 2D). Figure from Kipf and Welling [2017].

4.1 NODE EMBEDDING

Going back to Zachary’s Karate graph in Figure 4.1 (left), a standard clustering algorithm would detect four communities, shown by different colors. On the right side, a 2D embedding space is shown which represents nodes in the same graph, calculated using a recent node embedding technique, namely Graph Convolutional Networks (cf. Section 4.1.4). Clearly, the embedding has done a good job in preserving the structure of this graph, i.e., clusters and their relative positioning.

Representing graph nodes as numerical vectors¹ in continuous spaces can have many advantages, such as facilitating the visualization and analysis of global position of a node or a node’s neighbours. For instance, one can easily compute the “similarity” between two nodes or obtain a clustering of the nodes (similar to the one shown in the figure) by using a simple clustering technique based on distances in the space.

Traditional node representation techniques focused on hand-crafted features such as graph statistics (e.g., node degree), motifs [Milo et al., 2002], graph kernels [Vishwanathan et al., 2010], or carefully designed features to model sub-structures [Liben-Nowell and Kleinberg, 2003]. Like other feature-engineered models, this approach suffers from unreliable adaptability; features might not be applicable to a new domain and thinking of new features is an arduous process.

Recent years have seen a surge of techniques that try to bypass the need for feature engineering. In fact, the trend in graph representation is analogous to that of

¹For instance, the nodes in the Karate’s graph example are represented by a vector of two numbers.

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word modality: directly embed units as low-dimensional vectors into a continuous imaginary space without any pre-processing or feature extraction. In graph embedding, units are nodes (in contrast to words) and the objective is to preserve structural properties of the graph, such as node neighbourhood, rather than semantic or syntactic properties.

Graph embedding techniques can be broadly divided into three main categories:

1. Matrix factorization-based methods
2. Random-walk based algorithms
3. Graph neural networks

4.1.1 MATRIX FACTORIZATION METHODS

Similarly to word representations, conventional techniques to node representation all relied on extracting a set of pairwise similarity statistics for nodes coupled with a dimensionality reduction. For the case of words, co-occurrence counts are taken as a proxy for estimating the similarity of words. Given that co-occurrence matrices are generally large, a dimensionality reduction needs to be applied to compress word vectors into fewer number of dimensions (cf. Chapter 2). Similar statistical measures can be used for estimating node similarity in graphs. For instance, the existence of an edge between two nodes can denote their similarity. Therefore, the adjacency matrix of a graph (which expresses the edges in the graph) can be taken as a measure to estimate the pairwise similarities among the graph's nodes.

This class of techniques are referred to as Matrix Factorization (**MF**) because they represent graph properties, such as pairwise node similarity, as a matrix and compute embeddings for individual nodes by factorizing this matrix. The final goal in this domain is to compute embeddings for nodes such that the similarity between these embeddings (often computed as inner product) is highly correlated with the estimates given by graph-based node similarity measures. MF methods are generally inspired by dimensionality reduction techniques, such as Laplacian Eigenmaps [Belkin and Niyogi, 2003], Locality Preserving Projections [He and Niyogi, 2004], and Principal Component Analysis [Pearson, 1901].

The main distinguishing factor between different MF methods lies in their way of estimating the similarity between nodes. Various statistical measures have been proposed. Earlier ones usually model only first-order relationships between nodes, such as edges denoted by adjacency matrix used by Graph Factorization algorithm [Ahmed et al., 2013], whereas more recent works try to capture higher-order relationships in terms of some power of the adjacency matrix, such as GraRep [Cao et al., 2015], or Jaccard neighbourhood overlaps, such as HOPE [Ou et al., 2016a].

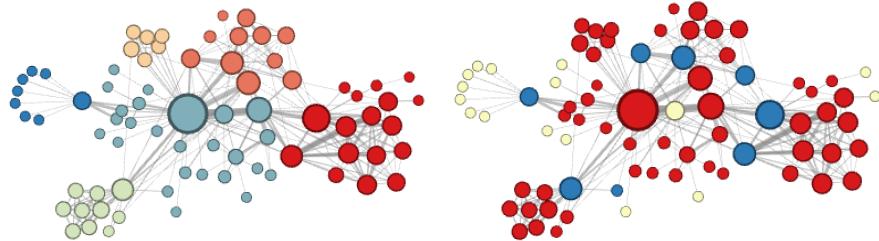


Figure 4.2: Representations learned for different configurations of Node2vec: left $q = 2$, right $q = 1$ ($p = 1$ for both settings). Graph nodes correspond to characters in the novel Les Misérables and edges connect coappearing characters. Representations are clustered using k-means; clusters shown by colors. Using controlled random walks in Node2vec, one can adjust the notion of similarity: macro or structural similarity in the left sub-figure and micro or homophily (or local) in the right sub-figure. Figure from [Grover and Leskovec, 2016].

4.1.2 RANDOM WALK METHODS

The measure of node similarity used by MF techniques is *deterministic* in that it relies on a set of fixed statistical features. MF is generally not scalable especially for very large networks for which gigantic matrices need to be constructed. Random Walk (**RW**) based methods are different in that they leverage a *stochastic* way of determining the similarity.

The core idea in this branch is to perform a series of truncated random walks on the graph, sampling nodes seen during each walk in order to transform the graph's structure into a collection of paths (node sequences). These paths can be viewed as artificial sentences. Similarly to natural language in which semantically similar words tend to co-occur frequently, artificial sentences carry information about similar (topologically related) vertices in the graph.

Earlier methods [Pilehvar et al., 2013, Hughes and Ramage, 2007] take the direct normalized visit probabilities as vectors. These RW-based node representations significantly outperformed conventional deterministic graph analysis approaches (such as normalized graph distance [Wu and Palmer, 1994]) when used for encoding semantic networks in a wide range of lexical semantic applications [Pilehvar and Navigli, 2015]. This was especially noticeable when the obtained representations were compared using a rank-based distance measure, instead of the widely-used Cosine distance [Pilehvar et al., 2013]. However, conventional RW-based measures suffer from a major limitation: high dimensionality.

Newer RW-based techniques employ neural networks to address the dimensionality issue. **DeepWalk** [Perozzi et al., 2014] and **Node2vec** [Grover and

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[Leskovec, 2016] are two prominent techniques in this branch. The core idea here is to benefit from the efficiency of Word2vec algorithms (cf. Section 3.2) for node representation. Word2vec receives sentences as its input and computes embeddings for its individual words. The gist of DeepWalk is to transform structure of a graph to a series of sequences, or artificial sentences whose “words” are nodes. Random walks fit very effectively in this framework. These sentences are then used as input to the Skip-gram model and embeddings for individual words (i.e., graph nodes) are computed.

Node2vec [Grover and Leskovec, 2016] is an extension of DeepWalk which provides a more flexible random walk that can control the notion of node similarity: homophily vs. structural. Figure 4.2 shows representations computed using different configurations of Node2vec. Specifically, Node2vec introduces two “bias” parameters which control the behaviour of random walks: p and q . The parameters control the tendency of the walk to stay in the neighbourhood or to leave that in exploration of other parts of the graph.

Imagine a walk moving from node u to v . The random choice of next node to visit from v is biased by an unnormalized transition probability α . With $\alpha = 1$ the walk visits a node which is at the same distance 1 of the starting node u . With probability $\alpha = 1/q$, the walk moves deeper in the network; setting q to a small value would bias the walk towards “outward” nodes, i.e., nodes that have distance 2 from starting node u . Parameter p performs a complementary role. The walk revisits the previous node, i.e., u , immediately with probability $1/p$. This keeps the walk close to the starting point; therefore, samples mostly comprise of nodes within a small locality. This gives a local view of the graph, capturing communities or homophily.

The two walk strategies can also be resembled by DFS (depth-first search) and BFS (breadth-first search). Setting p and q to model microscopic view of the neighbourhood is similar in merit to BFS. In contrast, DFS tends to move further away from the source, modeling the macroscopic view of the neighbourhood.

Structural roles. Most node embedding approaches that are covered in this book have the underlying assumption that nearby nodes in the graph should be associated with similar embeddings, i.e., they should be placed in close proximity of each other in the semantic space. We can think of tasks in which the “role” played by a node in a graph is at the center of attention rather than relative position. Node2vec provides a solution for this using the “bias” terms (see Figure 4.2). For instance, for a target task it might be important to model similarities between nodes that act as bridges between different communities, which might not necessarily be close to each other in the graph. Embedding “structural roles” of nodes has been an active field of research with several proposals, such

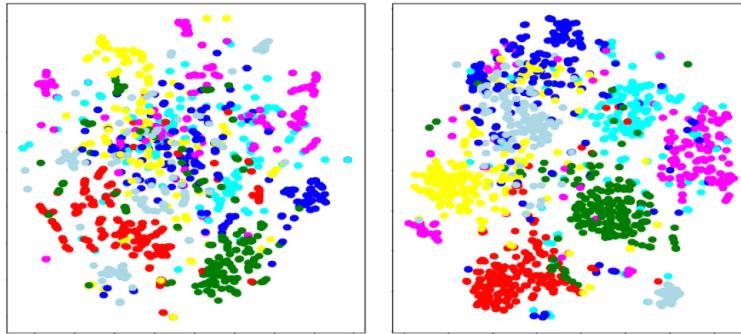


Figure 4.3: Embedded Cora citation network [McCallum et al., 2000] before (left) and after (right) enriching the graph with additional edges. The Cora dataset contains 2708 machine learning papers linked by citation relationships into a graph. Documents belong to 7 different categories, shown by different colors. Graph embedding carried out using DeepWalk and dimensionality reduction using t-SNE. Reprint from [Kartsaklis et al., 2018].

as Struc2vec [Ribeiro et al., 2017], GraphWave [Donnat et al., 2018], DRNE [Tu et al., 2018], xNetMF [Heimann et al., 2018].

It is also worthwhile to mention another technique, called **LINE** [Tang et al., 2015], which is not strictly RW-based, but closely related. LINE combines two different objectives to learn node embeddings: first-order and second-order. The first-order objective is analogous to the BFS search in Node2vec. The second-order objective forces nodes with similar neighbourhoods to have similar embeddings. The latter objective assumes that nodes with many common neighbours are probably similar to each other. In other words, if we take the neighbours of a node as its context, nodes with similar distributions over “contexts” are deemed to be similar.

4.1.3 INCORPORATING NODE ATTRIBUTES

It is usual for graph nodes to be associated with some attributes. Graphs in NLP are no exception. For instance, nodes (synsets) in WordNet are associated with various forms of textual data: synonymous terms, gloss (definition), and example sentences. The above techniques all make use of graph structure only, ignoring all these information.

Graph attributes, such as node content, can be used as a complementary source of information to the usually non-optimal structure of the networks. For instance, consider the synsets containing the frequently-used meanings of *com-*

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puter_monitor and *TV*. The two synsets are separated by 10 nodes in WordNet 3.0 which is a large distance given that the maximum depth of a nominal leaf node in WordNet is no more than 20. However, these are similar concepts that are also defined in WordNet with similar glosses.² A node embedding technique that merely takes into account the structure of WordNet would place these two semantically similar concepts at distance regions in the space. However, leveraging glosses would force these representations to look more similar, i.e., it pulls together the corresponding points in the space.

The non-optimality of graph structures has been highlighted in other works. For instance, Kartsaklis et al. [2018] showed for two different graphs that embedding the nodes based on structure only might not lead to desirable results. They proposed a technique for using node attributes for enriching networks with additional edges. They showed that an enriched graph can significantly improve the performance of DeepWalk in different NLP tasks. Figure 4.3 shows this improvement on one of the graphs, i.e., Cora citation network.

There are several variants of RW-based models that try to augment the structural data with other attributes, such as node content and label information. TriDNR [Pan et al., 2016], DDRW [Li et al., 2016], and DANE [Gao and Huang, 2018] are instances of such models. TriDNR is one of the most prominent techniques in this branch. The model follows RW-based methods and captures structural node relationships using random walks. However, it additionally exploits the content of nodes as well as edge labels for improving representations. The authors of TriDNR experimented with the document classification task in two citation networks in which papers are nodes and their titles are the content within nodes. They showed that significant improvements can be obtained by incorporating the additional attributes which are ignored by structure-only techniques such as DeepWalk and Node2vec.

Moreover, many of the graphs in NLP are actually hierarchies that are transformed into graphs. WordNet is an example of a hierarchical tree structure with additional lexical-semantic links. Synsets (nodes) at higher levels refer to more abstract concepts whereas they tend to be more specific and fine-grained deeper in the tree. Representing such structures as graphs (especially with non-directed edges) would discard all these semantic information. As a solution to this problem, Nickel and Kiela [2017] propose representing nodes as Poincaré balls³ which takes into account both similarity and the hierarchical structure of the taxonomy given as input⁴.

One might be interested in learning coarse node representations, i.e., to represent nodes at larger scales of relationships and their membership in hierarchies of

²TV: “an electronic device that receives television signals and displays them on a screen”, and *computer_monitor*: “a device that displays signals on a computer screen”

³A Poincaré ball is a hyperbolic space in which all points are inside the unit disk.

⁴WordNet is used as the reference taxonomy in the original work.

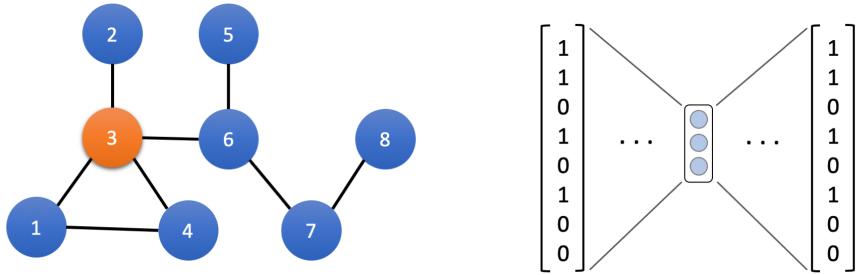


Figure 4.4: A toy graph with 8 nodes ($|V| = 8$) on the left and the general overview of an autoencoder-based node embedding technique on the right. For a target node (“3” in the figure) a context vector is extracted (simple adjacency statistics in this case). Autoencoder compresses the context vector into a much smaller embedding (with dimensionality $d \ll |V|$) for the corresponding node (shown at the middle). Autoencoder-based models mainly differ in their context vector or in the architecture of the autoencoder.

communities. Walklets [Perozzi et al., 2017] is an approach for multi-scale representation that facilitates this goal. The approach is similar to DeepWalk with the only difference that certain nodes are skipped from paths, in order to learn higher-scale relationships or coarse representations as if the focus area in graph is larger.

4.1.4 GRAPH NEURAL NETWORK METHODS

Given the dominance of deep learning, it is not surprising to expect node embedding techniques that are based on neural networks. In fact, despite the short age, there is an extensive branch of techniques that either directly make use of various deep learning models, such as autoencoders, for node representation or are inspired by ideas borrowed from deep learning, such as convolution operations.

This section provide a brief overview of the literature in neural network (NN) base graph embedding. We can be broadly classify NN-based models into two main categories: **autoencoder-based techniques** and **graph convolutional networks**.

Autoencoder-based models

Autoencoders are usually the first choice among neural network architectures for dimensionality reduction. The network, learns, in an unsupervised manner, to encode a given representation into a dense embedding from which it can reconstruct the same input. This property of autoencoders makes them a suitable candidate for substituting matrix factorization techniques.

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Figure 4.4 depicts the general procedure of a simple autoencoder-based node embedding model. Generally, these models comprise two stages in the pipeline. First, they analyze the structure of the network in order to extract a *context* vector for each node, which can characterize its local (or higher order) neighbourhood. Then, an autoencoder is used to compress the context vector into a dense low-dimensional embedding.

SDNE [Wang et al., 2016] and DNGR [Cao et al., 2016] are two of the most prominent models in this class. SDNE constructs the context vector simply based on the adjacency matrix (similar to what shown in Figure 4.4). DNGR leverages random walks for computing the context vector. Similarly to DeepWalk and Node2vec, DNGR carries out a series of truncated random walks to estimate pointwise mutual information between a target node and all other nodes in the graph. This is taken as a node’s context vector and fed for compression to the autoencoder network. DNGR is similar to ADW [Pilehvar et al., 2013] in the construction of context vector⁵. However, ADW simply takes the context vector, without any compression, as the final representation whereas DNGR compresses these into smaller embeddings.

One big limitation of autoencoder-based models lies in their global context vector, which is essentially equal in size to the number of nodes in the graph. This can make the procedure very expensive for large graphs. For instance, it might be manageable for relatively smaller graphs, such as WordNet with around 120K nodes, to be embedded using autoencoder-based models. However, for larger networks, such as BabelNet’s semantic network that has millions of nodes, autoencoder-based will certainly suffer from lack of **scalability** (very high number of parameters in the network).

Moreover, most of the node embedding techniques that are discussed so far are by design, transductive [Hamilton et al., 2017a], i.e., it is not straightforward to generate embeddings for new nodes (which are not seen during training) once the training is over, unless additional training is carried out. This can be limiting for evolving graphs, e.g., BabelNet (Live version) which is constantly updated with new concepts that are created by Wikipedians. A transductive model would fail at keeping up with the updates as the training has to be carried out from scratch for a new node embedding to be computed.

Convolution-based models

Driven by the ideas from computer vision, convolutional methods try to address the scalability and generalizability issues of previous techniques by resorting to local neighbourhood rather than global information. The main reason behind naming this branch as “convolutional” lies in the process of combining neighbouring nodes’

⁵ADW takes the Personalized PageRank vector for each node as its corresponding representation

4.2. KNOWLEDGE-BASED RELATION EMBEDDINGS 53

embeddings to construct a target embedding is analogous to convolution operation in computer vision CNNs [Hamilton et al., 2017a]. Graph Convolutional Networks [Kipf and Welling, 2017, GCN] and GraphSAGE [Hamilton et al., 2017b] are two of the most prominent models in this branch.

The basic idea is simple: to compute the embedding for a target node, look at the embeddings of neighbouring nodes. The neighbouring nodes are in turn embedded using their neighbours. This process is usually carried out in an iterative manner (the number of iterations is often referred to as “depth”).

More specifically, for a target node t and in each iteration, *aggregate* the embeddings of neighbouring nodes. The aggregation can be a simple element-wise mean, such as the case for GCNs. The resulting aggregated embedding is then *combined* with the previous estimate of t ’s embedding (from the previous iteration). GCNs use a weighed sum for this stage. Various models usually differ in how they define the aggregation and combination. For instance, GraphSAGE uses concatenation for its aggregation and test max-pooling networks and LSTMs as combination functions.

Thanks to the local nature of context lookup in convolutional models (as opposed to autoencoder-based models that require the global associations for each node with respect to all the other nodes in the graph) they can address both generalizability and scalability issues. An embedding for a new node can be easily computed based on learned aggregation and combination functions and by looking up the existing embeddings for neighbouring nodes.

4.2 KNOWLEDGE-BASED RELATION EMBEDDINGS

This section provides a review of those representation techniques targeting concepts and named entities from knowledge bases only. A large body of research in this area takes knowledge graphs (or semantic networks) as signals to construct representations of entities (and relations), specifically targeted to the knowledge base completion task⁶.

A pioneering work in this area is TransE [Bordes et al., 2013], a method to embed both entities and relations. In this model relations are viewed as translations which operate in the same vector space as entities. Given a knowledge base represented as a set of triples $\{(e_1, r, e_2)\}$, where e_1 and e_2 are entities and r the relation between them, the main goal is to approach the entities in a way that $\vec{e}_1 + \vec{r} \approx \vec{e}_2$ for all triples in the space (i.e., $\forall (e_1, r, e_2) \in N$). Figure 4.5 illustrates the main idea behind the model. This objective may be achieved by exploiting different learning architectures and constraints. In the original work of Bordes et al. [2013], the optimization is

⁶Given an incomplete knowledge base as input, the knowledge base completion task consists of predicting relations which were missing in the original resource.

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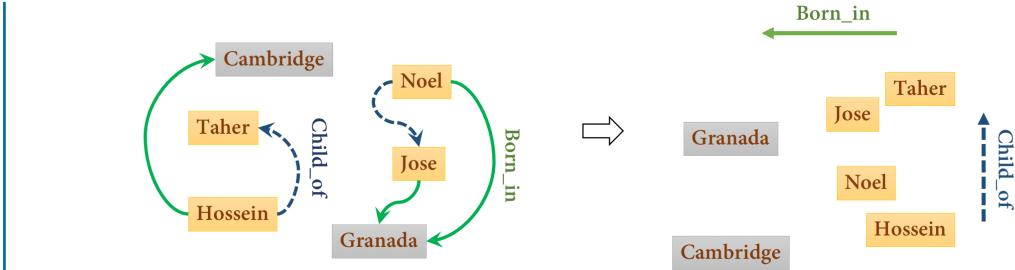


Figure 4.5: From a knowledge graph to entity and relation embeddings. Illustration idea is based on the slides of Weston and Bordes [2014].

carried out by stochastic gradient descent with an L_2 normalization of embeddings as an additional constraint. Following this underlying idea, various approaches have proposed improvements of different parts of the learning architecture:

- TransP [Wang et al., 2014b] is a similar model that provides improvements on the relational mapping by dealing with specific properties present in the knowledge graph.
- Lin et al. Lin et al. [2015] proposed to learn embeddings of entities and relations in separate spaces (TransR).
- Ji et al. [2015] introduced a dynamic mapping for each entity-relation pair in separated spaces (TransD).
- Luo et al. [2015] put forward a two-stage architecture using pre-trained word embeddings for initialization.
- A unified learning framework that generalize TransE and NTN [Socher et al., 2013a] was presented by Yang et al. [2015].
- Finally, Ebisu and Ichise [2018] discussed regularization issues from TransE and proposed TorusE, which benefits from a new regularization method solving TransE's regularization problems.

These have been some of the most relevant works on knowledge base embeddings in recent years, but given the multitude of papers on this topic, this review was by no means comprehensive. A broader overview of knowledge graph embeddings, including more in-depth explanations, is presented by Cai et al. [2018] or Nguyen [2017], the latter focusing on the knowledge base completion task.

4.3 UNSUPERVISED RELATION EMBEDDINGS

Modeling the interaction of a pair of concepts has been widely investigated since at least Turney [2005]. For instance, intuitively for a human the relation between *Paris* and *France*, and *Madrid* and *Spain* are similar, as they can both be integrated in a larger set of *capital-of* relations. These relations have been attempted to store in knowledge resources, as we showed in Section 2.3. However, the discrete nature of these relations have motivated a new field of study, which is their representation as part of continuous vector spaces. While there are approaches which do exactly this inside knowledge resources (see Section 4.2), it is hard to encode the whole nature of relational knowledge that human possesses in the well-defined relations available in existing knowledge resources.

Another way to model these relations between concepts is to leverage a text corpus, as is the case for word embeddings (see Chapter 3). In fact, a common way to model these relations is precisely via standard word embeddings [Mikolov et al., 2013d], often referred to as word analogies.

Word analogy. Word analogy has been very popular in NLP since Mikolov et al. [2013d]. In this work it was shown how Word2Vec word embeddings were able to capture linguistic relationships going beyond purely semantic similarity by exploiting word vector differences. For instance, *king* – *man* + *woman* would result in a vector that is close to *queen*.

Lately there have been some works aiming at understanding where these analogies come from. In general, it has been shown that word embeddings are not actually recovering general relations, but rather some specific ones for which similarity or proximity in the vector space plays an important role [Levy et al., 2014, Linzen, 2016, Rogers et al., 2017, Nissim et al., 2019]. For instance, Bouraoui et al. [2018] shows how word embeddings can capture relations such us superlative or capital of but then other relations cannot be retrieve by simple arithmetic operations from word embeddings. For a more detailed overview of the properties of word analogies, we would recommend the work of Allen and Hospedales [2019].

Co-occurrence based models. In one of the earlier works, Turney [2005] proposed a singular value decomposition (SVD) model. This model encoded different linguistic patterns of words, and how they are connected. A similar more recent work is that of Riedel et al. [2013], who represented word pairs as vectors, in this case combining co-occurrence statistics with information encoded in a knowledge graph. More recently, Jameel et al. [2018] proposed an unsupervised method for learning relation vectors which is inspired by the GloVe word embedding model. Their training

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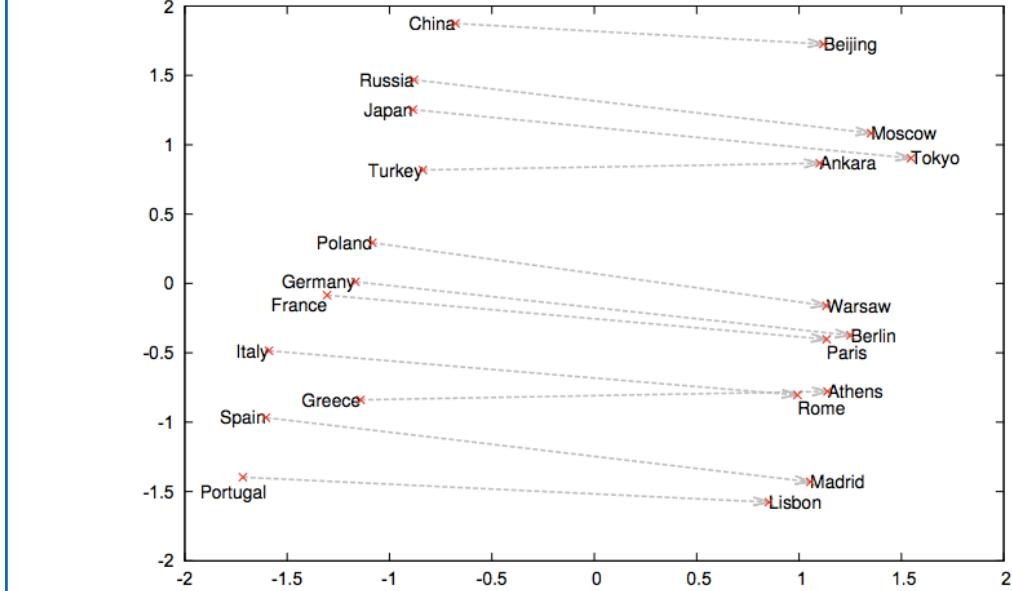


Figure 4.6: Word analogies in Word2Vec. Image borrowed from [Mikolov et al. \[2013c\]](#)).

objective is to learn vector representations r_{ab} of word pairs and vector representations \tilde{w}_c of context words, such that the dot product $r_{ab} \cdot \tilde{w}_c$ predicts the strength of association between occurrences of the context word c and the word pair (a, b) in a sentence. For this purpose, they considered a number of generalizations of PMI to three arguments. A simpler and more efficient alternative was proposed in [Espinosa-Anke and Schockaert \[2018\]](#), where relation vectors were learned by averaging the word vectors of the context words appearing in sentences that contain the word pair (a, b) and then using a conditional autoencoder. These averaging methods have been further refined by exploiting a latent variable models that assign probabilities to words as per their association to the given word pair [[Camacho-Collados et al., 2019](#)].

Predictive models. The aforementioned methods have the disadvantage that they can only learn relation vectors for pairs of words that co-occur in the same sentence sufficiently often. To address this, a number of methods have been proposed which learn word vectors that are aimed at modelling relational properties [[Washio and Kato, 2018b,a](#), [Joshi et al., 2019](#)]. Specifically, these works train a neural network that maps the concatenation of two word vectors $w_a \oplus w_b$ to a vector r_{ab} which represents the relation between the two corresponding words a and b . This network is

trained such that r_{ab} captures the contexts in which the word pair appears, where contexts correspond to learned vector encodings of dependency paths [Washio and Kato, 2018b] or LSTM-based neural encodings of surface patterns [Washio and Kato, 2018a, Joshi et al., 2019].

4.4 APPLICATIONS AND EVALUATION

This section provides a brief overview of the most commonly practised evaluation measures for graph embedding techniques. The discussion is divided based on the embedding type into node embedding and relation embedding. We also briefly discuss some of the applications of these embeddings.

4.4.1 NODE EMBEDDING

Evaluation of node embedding is usually centered around the notion of similarity between node embeddings. There are many evaluation setups, few of which are briefly discussed below.

- **Node classification.** One of the major applications of node embeddings is node classification, i.e., assigning labels to nodes based on the rules learned from the labeled subset nodes. This procedure can be viewed as label propagation in the graph. Given its supervised nature and ease of evaluation, node classification is often one of the first choices for evaluating node embeddings. For instance, one can view WordNet as a graph and compute embeddings for its nodes (synsets). Having domain labels for a set of synsets, the task would be to assign labels to unlabeled synsets.
- **Node clustering.** This is similar to node classification with the difference that labels are not pre-defined. Node clustering often involves computing similarities between nodes and grouping them based on their similarities. One application of node clustering would be to reduce the sense granularity of WordNet by grouping together those senses of a word that are similar.
- **Node ranking.** Given a target node, the task of node ranking consists of recommending the top K nodes according to a certain criteria, e.g., similarity. For instance, what are the three most semantically similar synsets to a given synset in WordNet. Node ranking has a wide range of applications, just to name a few, friend recommendation in social networks, question answering, and personalised advertisement.
- **Graph visualization.** The goal is to visualize a given graph on a low-dimensional space, usually 2D, to get a high-level overview of the properties of

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the graph. Nodes belonging to different categories can be shown with different colors. Figure 4.1 is an example of visualization. Given that node embeddings are usually of high dimensionality, which is not directly visualizable (> 3), it is necessary to carry out dimensionality reduction techniques, such as Principal Component Analysis [Jolliffe, 1986, PCA] and t-distributed Stochastic Neighbor Embedding [Maaten and Hinton, 2008, t-SNE] on the node embeddings, before visualizing the node embedding. Visualization can serve as a qualitative testbed for evaluating node embeddings. Moreover, it can have applications in other fields, such as software engineering, and biology, social network analysis, and bioinformatics [Herman et al., 2000].

- **Network compression.** *Reconstruction error* is a common way to quantify the ability of node embedding techniques in encoding structural information of a graph. According to this procedure, given the node embeddings computed for a graph, the graph is reconstructed. Reconstruction error is then computed as the difference between the original and reconstructed graphs. For instance, reconstruction can be viewed as predicting the edges of the original graph, and the error in this case can be directly computed as the accuracy of this prediction task. It is shown by different researchers [Wang et al., 2016, Ou et al., 2016b] that typical graphs can be reconstructed to a good accuracy from their node embeddings. This way, node embeddings can be considered as compressed forms of the topological information encoded in structure of graphs and can be effectively used to store them.

4.4.2 RELATION EMBEDDING

The main application of relation embeddings is link prediction. It is often the case that the richness of relations in an underlying semantic network has a direct impact on the performance of a model using that resource [Pilehvar et al., 2013, Agirre and Soroa, 2009]. Relations in networks are often constructed according to observed interactions between nodes. For instance, WordNet’s graph is usually enriched with relations extracted from manually disambiguated glosses. Therefore, given that glosses cannot contain all possible semantic relationships, the resulting semantic network can still be incomplete.

The task in link prediction consists of predicting missing edges in a graph. This can be extended to that of verifying existing edges in the graph, if the graph is expected to have spurious edges due to its construction procedure. Other applications of link prediction include friend suggestion in social friendship networks or biological network analysis [Goyal and Ferrara, 2018].

As far as unsupervised relation embeddings are concerned (cf. Section 4.3), their main application has been to model relationships of pairs of words. As more

4.4. APPLICATIONS AND EVALUATION 59

downstream applications, they have been integrated into pipelines for language understanding tasks such as reading comprehension [Joshi et al., 2019], text classification [Espinosa-Anke and Schockaert, 2018, Camacho-Collados et al., 2019] or relation extraction [Baldini Soares et al., 2019].

DRAFT

CHAPTER 5

Sense Embeddings

In this chapter we introduce those representations aiming to model unambiguous lexical meaning.¹ These representations emerge due to one of the main limitations of word-level representation techniques, which is the meaning conflation deficiency.

Meaning Conflation Deficiency. The prevailing objective of representing each word type as a single point in the semantic space has a major limitation: it ignores the fact that words can have multiple meanings and conflates all these meanings into a single representation. The work of Schütze [1998] is one of the earliest to identify the meaning conflation deficiency of word vectors. Having different (possibly unrelated) meanings conflated into a single representation can hamper the semantic understanding of an NLP system that uses these at its core. In fact, word embeddings have been shown to be unable in effectively capturing different meanings of a word, even when these meanings occur in the underlying training corpus [Yaghoobzadeh and Schütze, 2016]. The meaning conflation can have additional negative impacts on accurate semantic modeling, e.g., semantically unrelated words that are similar to different senses of a word are pulled towards each other in the semantic space [Neelakantan et al., 2014, Pilehvar and Collier, 2016]. For example, the two semantically-unrelated words *rat* and *screen* are pulled towards each other in the semantic space for their similarities to two different senses of *mouse*, i.e., rodent and computer input device. See Figure 5.1 for an illustration. Moreover, the conflation deficiency violates the triangle inequality of euclidean spaces, which can reduce the effectiveness of word space models [Tversky and Gati, 1982].

In order to alleviate this deficiency, a new direction of research has emerged over the past years, which tries to directly model individual meanings of words. In this survey we focus on this new branch of research, which has some similarities and peculiarities with respect to word representation learning. There are two main branches to model senses, unsupervised (Section 5.1) or knowledge-based (Section 5.2). In Section 5.3 we additionally present common evaluation procedures and applications of such representations.

¹This chapter is largely inspired by our recent survey [Camacho-Collados and Pilehvar, 2018] - Sections 3 and 4.

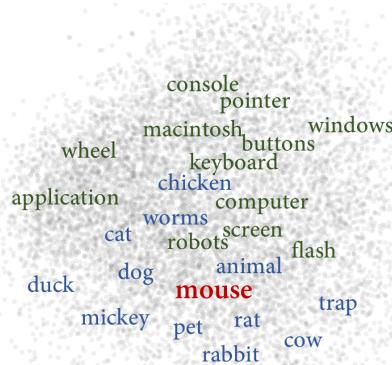


Figure 5.1: An illustration of the meaning conflation deficiency in a 2D semantic space around the ambiguous word *mouse* (dimensionality was reduced using PCA; visualized with the embedding projector of Tensorflow). Having the word, with its different meanings, represented as a single point (vector) results in pulling together of semantically unrelated words, such as *computer* and *rabbit*.

5.1 UNSUPERVISED SENSE EMBEDDINGS

Unsupervised sense representations are constructed on the basis of information extracted from text corpora only. Word sense induction, i.e., automatic identification of possible meanings of words, lies at the core of these techniques. An unsupervised model induces different senses of a word by analysing its contextual semantics in a text corpus and represents each sense based on the statistical knowledge derived from the corpus. Depending on the type of text corpus used by the model, we can split unsupervised sense representations into two broad categories: (1) techniques that exploit monolingual corpora only (Section 5.1.1), and (2) those exploiting multilingual corpora (Section 5.1.2).

5.1.1 SENSE REPRESENTATIONS EXPLOITING MONOLINGUAL CORPORA

This section reviews sense representation models that use unlabeled monolingual corpora as their main resource. These approaches can be divided into two main groups:

1. **clustering-based** (or **two-stage**) models [Van de Cruys et al., 2011, Erk and Padó, 2008, Liu et al., 2015a], which first induce senses and then learn representations for these (Section 5.1.1),

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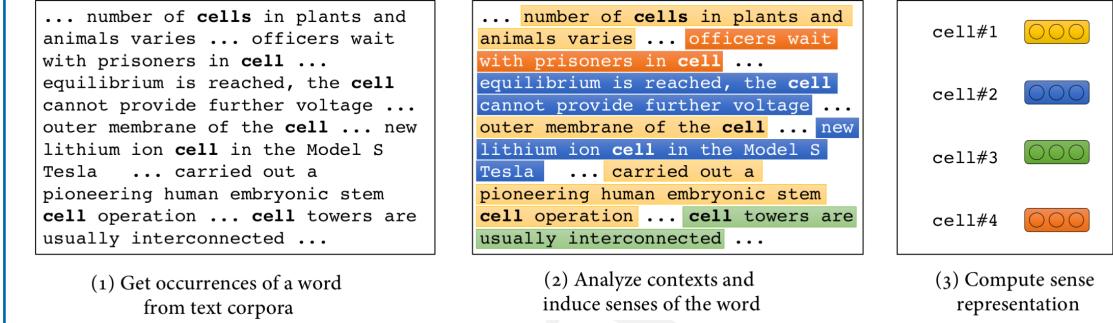


Figure 5.2: Unsupervised sense representation techniques first induce different senses of a given word (usually by means of clustering occurrences of that word in a text corpus) and then compute representations for each induced sense.

2. **joint training** [Li and Jurafsky, 2015, Qiu et al., 2016], which perform the induction and representation learning together (Section 5.1.1).

Two-Stage Models

The *context-group discrimination* of Schütze [1998] is one of the pioneering works in sense representation. The approach was an attempt to *automatic* word sense disambiguation in order to address the knowledge-acquisition bottleneck for sense annotated data [Gale et al., 1992] and reliance on external resources. The basic idea of context-group discrimination is to automatically induce senses from contextual similarity, computed by **clustering** the contexts in which an ambiguous word occurs. Specifically, each context C of an ambiguous word w is represented as a context vector \vec{v}_C , computed as the centroid of its content words' vectors \vec{v}_c ($c \in C$). Context vectors are computed for each word in a given corpus and then clustered into a predetermined number of clusters (context groups) using the Expectation Maximization algorithm [Dempster et al., 1977, EM]. Context groups for the word are taken as representations for different senses of the word. Despite its simplicity, the clustering-based approach of Schütze [1998] constitutes the basis for many of the subsequent techniques, which mainly differed in their representation of context or the underlying clustering algorithm. Figure 5.2 depicts the general procedure followed by the two-stage unsupervised sense representation techniques.

Given its requirement for computing independent representations for all individual contexts of a given word, the context-group discrimination approach is not easily scalable to large corpora. Reisinger and Mooney [2010] addressed this by directly clustering the contexts, represented as feature vectors of unigrams, instead of modeling contexts as vectors. The approach can be considered as the first

new-generation sense representation technique, which is often referred to as *multi-prototype*. In this specific work, contexts were clustered using Mixtures of von Mises-Fisher distributions (movMF) algorithm. The algorithm is similar to k-means but permits controlling the semantic breadth using a per-cluster concentration parameter which would better model skewed distributions of cluster sizes.

Similarly, Huang et al. [2012] proposed a clustering-based sense representation technique with three differences: (1) context vectors are obtained by a idf-weighted averaging of their word vectors; (2) spherical k-means is used for clustering; and (3) most importantly, occurrences of a word are labeled with their cluster and a second pass is used to learn sense representations. The idea of two-pass learning has also been employed by Vu and Parker [2016] for another sense representation modeling architecture.

Sense representations can also be obtained from semantic networks. For instance, Pelevina et al. [2016] constructed a semantic graph by connecting each word to the set of its semantically similar words. Nodes in this network were clustered using the Chinese Whispers algorithm [Biemann, 2006] and senses were induced as a weighted average of words in each cluster. A similar sense induction technique was employed by Sense-aware Semantic Analysis [Wu and Giles, 2015, SaSA]. SaSA follows Explicit Semantic Analysis [Gabrilovich and Markovitch, 2007, ESA] by representing a word using Wikipedia concepts. Instead of constructing a nearest neighbour graph, a graph of Wikipedia articles is built by gathering all related articles to a word w and clustering them. The sense induction step is then performed on the semantic space of Wikipedia articles.

Joint Models

The clustering-based approach to sense representation suffers from the limitation that clustering and sense representation are done independently from each other and, as a result, the two stages do not take advantage from their inherent similarities. The introduction of embedding models was one of the most revolutionary changes to vector space models of word meaning. As a closely related field, sense representations did not remain unaffected. Many researchers have proposed various extensions of the Skip-gram model [Mikolov et al., 2013a] which would enable the capture of sense-specific distinctions. A major limitation of the two-stage models is their computational expensiveness². Thanks to the efficiency of embedding algorithms and their unified nature (as opposed to the two-phase nature of more conventional techniques) these techniques are generally efficient. Hence, many of the recent techniques have relied on embedding models as their base framework.

²For instance, the model of Huang et al. [2012] took around one week to learn sense embeddings for a 6,000 subset of the 100,000 vocabulary on a corpus of one billion tokens [Neelakantan et al., 2014].

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Neelakantan et al. [2014] was the first to propose a multi-prototype extension of the Skip-gram model. Their model, called Multiple-Sense Skip-Gram (MSSG), is similar to earlier work in that it represents the context of a word as the centroid of its words' vectors and clusters them to form the target word's sense representation. Though, the fundamental difference is that clustering and sense embedding learning are performed jointly. During training, the intended sense for each word is dynamically selected as the closest sense to the context and weights are updated only for that sense. In a concurrent work, Tian et al. [2014] proposed a Skip-gram based sense representation technique that significantly reduced the number of parameters with respect to the model of Huang et al. [2012]. In this case, word embeddings in the Skip-gram model are replaced with a finite mixture model in which each mixture corresponds to a prototype of the word. The EM algorithm was adopted for the training of this multi-prototype Skip-gram model.

Liu et al. [2015b] argued that the above techniques are limited in that they consider only the local context of a word for inducing its sense representations. To address this limitation, they proposed Topical Word Embeddings (TWE) in which each word is allowed to have different embeddings under different topics, where topics are computed globally using latent topic modelling [Blei et al., 2003a]. Three variants of the model were proposed: (1) TWE-1, which regards each topic as a pseudo word, and learns topic embeddings and word embeddings separately; (2) TWE-2, which considers each word-topic as a pseudo word, and learns topical word embeddings directly; and (3) TWE-3, which assigns distinct embeddings for each word and each topic and builds the embedding of each word-topic pair by concatenating the corresponding word and topic embeddings. Various extensions of the TWE model have been proposed. The Neural Tensor Skip-gram (NTSG) model [Liu et al., 2015a] applies the same idea of topic modeling for sense representation but introduces a tensor to better learn the interactions between words and topics. Another extension is MSWE [Nguyen et al., 2017], which argues that multiple senses might be triggered for a word in a given context and replaces the selection of the most suitable sense in TWE by a mixture of weights that reflect different association degrees of the word to multiple senses in the context.

These joint unsupervised models, however, suffer from two limitations. First, for ease of implementation, most unsupervised sense representation techniques assume a fixed number of senses per word. This assumption is far from being realistic. Words tend to have a highly variant number of senses, from one (monosemous) to dozens. In a given sense inventory, usually, most words are monosemous. For instance, around 80% of words in WordNet 3.0 are monosemous, with less than 5% having more than 3 senses. However, ambiguous words tend to occur more frequently in a real text which slightly smooths the highly skewed distribution of words

# Senses	2	3	4	5	6	7	8	9	10	11	12	≥ 12
Nouns	22%	17%	14%	13%	9%	7%	4%	4%	3%	3%	1%	3%
Verbs	15%	16%	14%	13%	9%	7%	5%	4%	4%	3%	1%	9%
Adjectives	23%	19%	15%	12%	8%	5%	2%	3%	3%	1%	2%	6%

Table 5.1: Distribution of words per number of senses in the SemCor dataset (words with frequency < 10 were pruned).

across polysemy. Table 5.1 shows the distribution of word types by their number of senses in SemCor [Miller et al., 1993], one of the largest available sense-annotated datasets which comprises around 235,000 semantic annotations for thousands of words. The skewed distribution clearly shows that word types tend to have varying number of senses in a natural text, as also discussed in other studies [Piantadosi, 2014, Bennett et al., 2016, Pasini and Navigli, 2018].

Second, a common strand of most unsupervised models is that they extend the Skip-gram model by replacing the conditioning of a word to its context (as in the original model) with an additional conditioning on the intended senses. However, the context words in these models are not disambiguated. Hence, a sense embedding is conditioned on the word embeddings of its context.

In the following we review some of the approaches that are directly targeted at addressing these two limitations of the joint unsupervised models described above:

1. **Dynamic polysemy.** A direct solution to the varying polysemy problem of sense representation models would be to set the number of senses of a word as defined by an external sense inventory. The Skip-gram extension of Nieto Piña and Johansson [2015] follows this procedure. However, by taking external lexicons as groundtruth the approach suffers from two main limitations. First, the model is unable to handle words that are not defined in the lexicon. Second, the model assumes that the sense distinctions defined by the underlying text match those specified by the lexicon, which might not be necessarily true. In other words, not all senses of a word might have occurred in the text or the lexicon might not cover all the different intended senses of the word in the underlying text. A better solution would involve dynamic induction of senses from the underlying text. Such a model was first implemented in the non-parametric MSSG (NP-MSSG) system of Neelakantan et al. [2014]. The model applies the online non-parametric clustering procedure of Meyerson [2001] to the task by creating a new sense for a word type only if its similarity (as computed using the current context) to existing senses for the word is less than a parameter λ . AdaGram [Bartunov et al., 2016] improves this dynamic behaviour by a more

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principled nonparametric Bayesian approach. The model, which similarly to previous works builds on Skip-gram, assumes that the polysemy of a word is proportional to its frequency (more frequent words are probably more polysemous).

2. **Pure sense-based models.** Ideally, a model should model the dependency between sense choices in order to address the ambiguity from context words. Qiu et al. [2016] addressed this problem by proposing a pure sense-based model. The model also expands the disambiguation context from a small window (as done in the previous works) to the whole sentence. MUSE [Lee and Chen, 2017] is another Skip-gram extension that proposes pure sense representations using reinforcement learning. Thanks to a linear-time sense sequence decoding module, the approach provides a more efficient way of searching for sense combinations.

5.1.2 SENSE REPRESENTATIONS EXPLOITING MULTILINGUAL CORPORA

Sense distinctions defined by a sense inventory such as WordNet might not be optimal for some downstream applications, such as Machine Translation (MT). Given that ambiguity does not necessarily transfer across languages, sense distinctions for MT should ideally be defined based on the translational differences across a specific language pair. The usual approach to do this is to cluster possible translations of a source word in the target language, with each cluster denoting a specific sense of the source word.

Such translation-specific sense inventories have been used extensively in MT literature [Ide et al., 2002, Carpuat and Wu, 2007, Bansal et al., 2012, Liu et al., 2018]. The same inventory can be used for the creation of sense embeddings that are suitable for MT. Guo et al. [2014] induced a sense inventory in the same manner by clustering words' translations in parallel corpora. Words in the source language were tagged with their corresponding senses and the automatically annotated data was used to compute sense embeddings using standard word embedding techniques. Ettinger et al. [2016] followed the same sense induction procedure but used the retrofitting-based sense representation of Jauhar et al. [2015]³, by replacing the standard sense inventory used in the original model (WordNet) with a translation-specific inventory.

Similarly, Šuster et al. [2016] exploited translation distinctions as supervisory signal in an autoencoder for inducing sense representations. At the encoding stage, the discrete-state autoencoder assigns a sense to the target word and during decoding

³See Section 5.2 for more details on this model.

recovers the context given the word and its sense. At training time, the encoder uses words as well as their translations (from aligned corpora). This bilingual model was extended by [Upadhyay et al. \[2017\]](#) to a multilingual setting, in order to better benefit from multilingual distributional information.

5.2 KNOWLEDGE-BASED SENSE EMBEDDINGS

This section provides an overview of the state of the art in knowledge-based sense representations. These representations are usually obtained as a result of *de-conflating* a word into its individual sense representations, as defined by an external sense inventory. Figure 5.3 depicts the main workflow for knowledge-based sense vector representation modeling techniques.

Word Sense Disambiguation. Word Sense Disambiguation (WSD) is a task which is closely related to the meaning conflation deficiency. WSD has been a long-standing task in NLP and AI [[Navigli, 2009](#)], dating back to the first half of the 20th century where it was viewed as a key intermediate task for machine translation [[Weaver, 1955](#)]. Given a word in context, the task of WSD consists of associating the word with its most appropriate meaning as defined by a sense inventory. For example, in the sentence “My *mouse* was broken, so I bought a new one yesterday.”, *mouse* would be associated with its *computer device* meaning, assuming an existing entry for such sense in the pre-defined sense inventory.

WSD has been catalogued as an AI-complete problem [[Mallery, 1988](#), [Navigli, 2009](#)] and its challenges (still present nowadays) are manifold: sense granularity, corpus domain or the representation of word senses (topic addressed in this survey), to name a few. In addition, the fact that WSD relies on knowledge resources poses additional challenges such as the creation of such resources and the construction of sense-annotated corpora. All of these represent a very expensive and time-consuming effort, which needs to be re-done for different resources and languages, and updated over time. This causes the so-called knowledge-acquisition bottleneck [[Gale et al., 1992](#)].

The knowledge resources and sense inventories traditionally used in WSD have been associated with entries on a standard dictionary, with WordNet [[Miller et al., 1993](#)] being the de-facto sense inventory for WSD. Nevertheless, other machine-readable structures can be (and are) considered in practice. For example, Wikipedia, which is constantly being updated, can be viewed as a sense inventory where each entry corresponds to a different concept or entity [[Mihalcea and Csomai, 2007](#)]. Senses can even be induced automatically from a corpus using unsupervised methods, a task known as word sense induction or discrimination.

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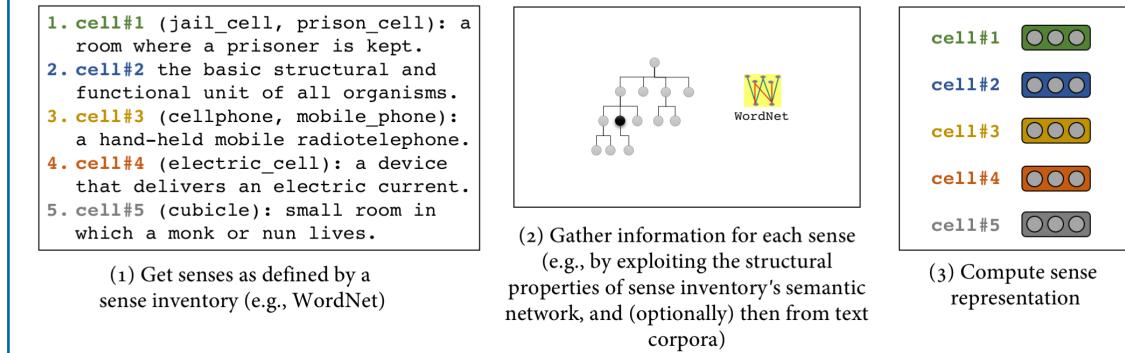


Figure 5.3: Knowledge-based sense representation techniques take sense distinctions for a word as defined by an external lexical resource (sense inventory). For each sense, relevant information is gathered and a representation is computed.

Methods to perform WSD can be roughly divided into two classes: supervised [Zhong and Ng, 2010, Iacobacci et al., 2016, Yuan et al., 2016, Raganato et al., 2017b, Luo et al., 2018] and knowledge-based [Lesk, 1986, Banerjee and Pedersen, 2002, Agirre et al., 2014, Moro et al., 2014, Tripodi and Pelillo, 2017, Chaplot and Salakhutdinov, 2018]. While supervised methods make use of sense-annotated corpora, knowledge-based methods exploit the structure and content of the underlying knowledge resource (e.g. definitions or a semantic network).^a Currently, supervised methods clearly outperform knowledge-based systems [Raganato et al., 2017a]; but, as mentioned earlier, they heavily rely on the availability of sense-annotated corpora, which is generally scarce.

In this book we will not go into further details of WSD. For a comprehensive historical overview of WSD we would recommend the survey of Navigli [2009], and a more recent analysis of current methods can be found in the empirical comparison of Raganato et al. [2017a].

^aSome methods can also be categorized as hybrid, as they make use of both sense-annotated corpora and knowledge resources, e.g., the gloss-augmented model of Luo et al. [2018].

The learning signal for these techniques vary, but in the main two different types of information available in lexical resources are leveraged: textual definitions (or *glosses*) and semantic networks.

Textual definitions are used as main signals for initializing sense embeddings by several approaches. Chen et al. [2014] proposed an initialization of word sense embeddings by averaging pre-trained word embeddings trained on text corpora. Then, these initialized sense representations are utilized to disambiguate a large

5.2. KNOWLEDGE-BASED SENSE EMBEDDINGS 69

corpus. Finally, the training objective of Skip-gram from Word2vec [Mikolov et al., 2013a] is modified in order to learn both word and sense embeddings from the disambiguated corpus. In contrast, Chen et al. [2015] exploited a convolutional neural network architecture for initializing sense embeddings using textual definitions from lexical resources. Then, these initialized sense embeddings are fed into a variant of the Multi-sense Skip-gram Model of Neelakantan et al. [2014] (see Section 5.1.1) for learning knowledge-based sense embeddings. Finally, in Yang and Mao [2016] word sense embeddings are learned by exploiting an adapted Lesk⁴ algorithm [Vasilescu et al., 2004] over short contexts of word pairs.

A different line of research has experimented with the graph structure of lexical resources for learning knowledge-based sense representations. As explained in Section 2.3, many of the existing lexical resources can be viewed as **semantic networks** in which nodes are concepts and edges represent the relations among concepts. Semantic networks constitute suitable knowledge resources for disambiguating large amounts of text [Agirre et al., 2014, Moro et al., 2014]. Therefore, a straightforward method to learn sense representations would be to automatically disambiguate text corpora and apply a word representation learning method on the resulting sense-annotated text [Iacobacci et al., 2015]. Following this direction, Mancini et al. [2017] proposed a shallow graph-based disambiguation procedure and modified the objective functions of Word2vec in order to simultaneously learn word and sense embeddings in a shared vector space. The objective function is in essence similar to the objective function proposed by Chen et al. [2014] explained before, which also learns both word and sense embeddings in the last step of the learning process.

Similarly to the post-processing of word embeddings by using knowledge resources (see Section 3.4), recent works have made use of pre-trained word embeddings not only for improving them but also de-conflating them into senses. Approaches that **post-process pre-trained word embeddings** for learning sense embeddings are listed below:

1. One way to obtain sense representations from a semantic network is to directly apply the Personalized PageRank algorithm [Haveliwala, 2002], as done by Pilehvar and Navigli [2015]. The algorithm carries out a set of random graph walks to compute a vector representation for each WordNet synset (node in the network). Using a similar random walk-based procedure, Pilehvar and Collier [2016] extracted for each WordNet word sense a set of *sense biasing words*. Based on these, they put forward an approach, called DeConf, which takes a pre-trained word embeddings space as input and adds a set of sense embeddings (as defined by WordNet) to the same space. DeConf achieves this by push-

⁴The original Lesk algorithm [Lesk, 1986] and its variants exploit the similarity between textual definitions and a target word's context for disambiguation.

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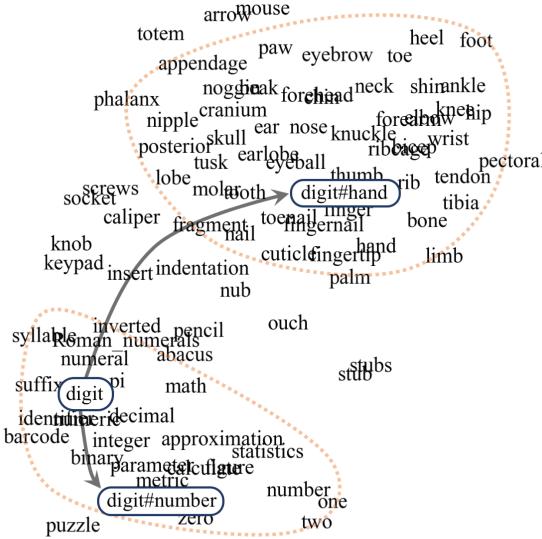


Figure 5.4: A mixed semantic space of words and word senses. DeConf [Pilehvar and Collier, 2016] introduces two new points in the word embedding space, for the *mathematical* and *body part* senses of the word *digit*, resulting in the mixed space.

ing a word’s embedding in the space to the region occupied by its corresponding sense biasing words (for a specific sense of the word). Figure 5.4 shows the word *digit* and its induced *hand* and *number* senses in the vector space.

2. Jauhar et al. [2015] proposed an extension of *retrofitting*⁵ [Faruqui et al., 2015] for learning representations for the senses of the underlying sense inventory (e.g., WordNet). They additionally presented a second approach which adapts the training objective of Word2vec to include senses within the learning process. The training objective is optimized using EM.
3. Johansson and Pina [2015] post-processed pre-trained word embeddings through an optimization formulation with two main constraints: polysemous word embeddings can be decomposed as combinations of their corresponding sense embeddings and sense embeddings should be close to their neighbours in the semantic network. A Swedish semantic network, SALDO [Borin et al., 2013], was used in their experiments, although their approach may be directly extensible to different semantic networks as well.

⁵See Section 3.4 for more information on retrofitting.

- Finally, AutoExtend [Rothe and Schütze, 2015] is another method using pre-trained word embeddings as input. In this case, they put forward an autoencoder architecture based on two main constraints: a word vector corresponds to the sum of its sense vectors and a synset to the sum of its lexicalizations (senses). For example, the vector of the word *crane* would correspond to the sum of the vectors for its senses $crane_n^1$, $crane_n^2$ and $crane_v^1$ (using WordNet as reference). Similarly, the vector of the synset defined as “arrange for and reserve (something for someone else) in advance” in WordNet would be equal to the sum of the vectors of its corresponding senses *reserve*, *hold* and *book*. Equation 5.1 displays these constraints mathematically:

$$\vec{w} = \sum_{i=1}^n \vec{s}_i; \quad \vec{y} = \sum_{j=1}^m \vec{s}_j, \quad (5.1)$$

where s_i and s_j refer to the senses of word w and synset y , respectively.

Concept and Entity Representations. In addition to these methods representing senses as represented in a sense inventory, other models combine cues from text corpora and knowledge resources to learn representations for concepts and entities (e.g. WordNet synsets or Wikipedia entities).^a Given its semi-structured nature and the textual content provided, Wikipedia has been the main source for these kind of representations. While most approaches make use of Wikipedia-annotated corpora as their main source to learn representations for Wikipedia concepts and entities [Wang et al., 2014a, Sherkat and Milios, 2017, Cao et al., 2017], the combination of knowledge from heterogeneous resources like Wikipedia and WordNet has also been explored [Camacho-Collados et al., 2016].^b

Given their hybrid nature, these models can easily be used in textual applications as well. A straightforward application is word or named entity disambiguation, for which the embeddings can be used as initialization in the embedding layer on a neural network architecture [Fang et al., 2016, Eshel et al., 2017] or used directly as a knowledge-based disambiguation system exploiting semantic similarity [Camacho-Collados et al., 2016].

^aFor those methods that rely solely on the relational information of knowledge bases, please refer to Section 4.1.

^bThe combination of Wikipedia and WordNet relies on the multilingual mapping provided by BabelNet (see Section 2.3.3 for more information about BabelNet).

5.3 EVALUATION AND APPLICATION

The main reason behind the existence of sense representations is that they are a solution to the meaning conflation deficiency of word representations. Given that sense representations are often considered as a specialised form of word embeddings, the sense representation models have often been evaluated on intrinsic benchmarks designed for words (see Chapter 5 for an overview). This has also been driven by the fact that there are not many reliable intrinsic benchmarks for evaluating sense representations.

In order to adapt intrinsic word similarity benchmarks to evaluating sense embeddings, various strategies have been proposed [Reisinger and Mooney, 2010]. Among these, the most popular is to take the most similar pair of senses across the two words [Resnik, 1995, Pilehvar and Navigli, 2015, Mancini et al., 2017], also known as *MaxSim*:

$$\text{sim}(w_1, w_2) = \max_{s_1 \in S_{w_1}, s_2 \in S_{w_2}} \cos(\vec{s}_1, \vec{s}_2) \quad (5.2)$$

where S_{w_i} is a set including all senses of w_i and \vec{s}_i represents the sense vector representation of the sense s_i . Another strategy, known as *AvgSim*, simply averages the pairwise similarities of all possible senses of w_1 and w_2 . Cosine similarity (\cos) is the most prominent metric for computing the similarity between sense vectors.

In all these benchmarks, words are paired in isolation. However, we know that for a specific meaning of an ambiguous word to be triggered, the word needs to appear in particular contexts. In fact, Kilgarriff [1997] argued that representing a word with a fixed set of senses may not be the best way for modelling word senses but instead, word senses should be defined according to a given context. To this end, Huang et al. [2012] presented a different kind of similarity dataset in which words are provided with their corresponding contexts. The task consists of assessing the similarity of two words by taking into consideration the contexts in which they occur. The dataset is known as Stanford Contextual Word Similarity (SCWS) and has been established as one of the main intrinsic evaluations for sense representations.

A pre-disambiguation step is required to leverage sense representations in the contextual word similarity task. Simple similarity measures such as *MaxSimC* or *AvgSimC* can be used; however, they cannot incorporate the context of words. The more suitable choice of strategy for this setting is either *MaxSim* and *AvgSim*, *MaxSimC* and *AvgSimC* which allow entering context into the similarity computation. First, the confidence for selecting the most appropriate sense within the sentence is computed (for instance by computing the average of word embeddings from the context and selecting the sense which is closest to the average context vector in terms of cosine similarity). Then, the final score corresponds to the similarity be-

5.3. EVALUATION AND APPLICATION 73

tween the selected senses (i.e., MaxSimC) or to a weighted average among all senses (i.e., AvgSimC).

However, even though sense representations have generally outperformed word-based models on intrinsic evaluations, the simple strategies used to disambiguate the input text may not have been optimal. In fact, it has been recently shown that the improvements of sense-based models in word similarity tasks using AvgSim may not be due to accurate meaning modeling but to related artifacts such as sub-sampling, which had not been controlled for [Dubossarsky et al., 2018].

The Word-in-Context (WiC) dataset [Pilehvar and Camacho-Collados, 2018] is one of the very few existing intrinsic benchmarks specifically designed for evaluating sense representations. WiC is framed as a binary classification task which alleviates the dependency on specific sense inventories. Each instance in WiC has a target word w , either a verb or a noun, for which two contexts are provided. Each of these contexts triggers a specific meaning of w . The task is to identify if the occurrences of w in the two contexts correspond to the same meaning or not. In fact, the dataset can also be viewed as an application of Word Sense Disambiguation that alleviates dependency on specific sense inventories.

Extrinsic evaluation of sense representations is very similar to that for word representations (cf. Section 3.6.2). The main distinguishing difference is that in the former, the input needs to be disambiguated to allow the integration of sense representations. This introduces another source of uncontrolled noise especially given the non-optimality of disambiguation techniques. Some of the most common tasks that have been used as extrinsic evaluation are text categorization and sentiment analysis [Liu et al., 2015b, Li and Jurafsky, 2015, Pilehvar et al., 2017], document similarity [Wu and Giles, 2015], and word sense induction [Pelevina et al., 2016, Panchenko et al., 2017] and disambiguation [Chen et al., 2014, Rothe and Schütze, 2015, Camacho-Collados et al., 2016, Peters et al., 2018].

CHAPTER 6

Contextualized Embeddings

This chapter provides an introduction to *contextualized word (CW) embeddings*. CW can be considered as the new generation of word (and sense) embeddings. The distinguishing factor here is the sensitiveness of a word's representation to the context: a target word's embedding can change depending on the context in which it appears. These *dynamic* embeddings alleviate many of the issues associated with *static* word embeddings and provide reliable means for capturing semantic and syntactic properties of natural language in context. Despite their young age, contextualized word embeddings have provided significant gains in almost any downstream NLP task to which they have been applied.

6.1 THE NEED FOR CONTEXTUALIZATION

Since their introduction, pre-trained word embeddings have dominated the field of semantic representation. They have been a key component in most neural natural language processing systems. Usually, an NLP system is provided with large pre-trained word embeddings for all the words in the vocabulary of the target language.¹ At the input layer, the system looks up the embedding for a given word and feeds the corresponding embedding to the subsequent layers (as opposed to a one-hot representation). Figure 6.1(a) depicts the general architecture for such a system. Moving from hard-coded one-hot representations to a continuous word embedding space usually results in improved generalisation power of the system, hence improved performance.

However, pre-trained word embeddings, such as Word2vec and GloVe, compute a single *static* representation for each word. The representation is fixed; it is independent from the context in which the word appears. In our example in Figure 6.1(a), the same embedding would be used at the input layer for *cell* even if the word was used in different contexts that would have triggered its other meanings, e.g., “the cells of a honeycomb”, “mobile cell”, and “prison cell”.

¹For instance, the widely-used Google News Word2vec embeddings has a vocabulary of three million words: <https://code.google.com/archive/p/word2vec/>

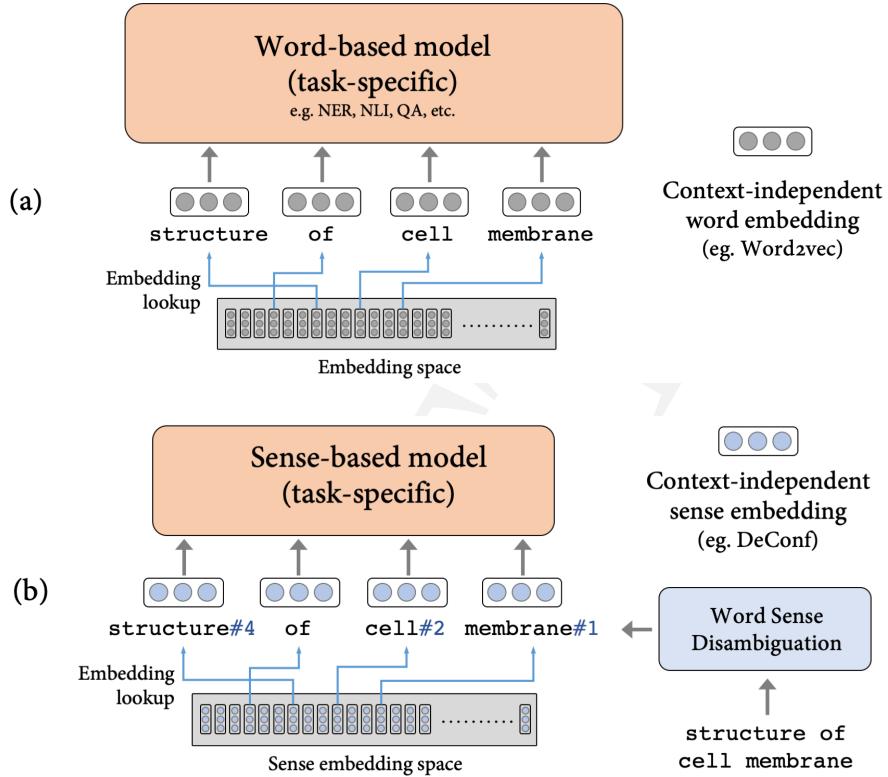


Figure 6.1: Context-independent (static) embeddings are fixed points in the semantic space: they do not change, irrespective of the context in which the target word appears. In the word-based model (a) For each input word, the static embedding is looked up from a pre-trained semantic space. Embeddings are introduced as features, usually in the input layer. In the sense based model (b), words are first disambiguated before being input to the system, and the corresponding sense embeddings are passed to the model.

Static semantic representations suffer from two important limitations: (1) ignoring the role of context in triggering specific meanings of words is certainly an oversimplification of the problem; this is not the way humans interpret meanings of words in texts; (2) due to restricting the semantic barriers to individual words, it is difficult for the model to capture higher order semantic phenomena, such as compositionality and long-term dependencies. Therefore, the static word-based representation of words can substantially hamper the ability of NLP systems in understanding the semantics of the input text. In this setting, all the load of deriving meaning from

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a sequence of words is on the shoulders of the main system, which has to deal with ambiguity, syntactic nuances, agreement, negation, etc.

Knowledge-based sense representations (discussed in Chapter 5) can partly address the first issue. The distinct representations they provide for specific meanings of polysemous words enable the model to have a clear interpretation of the intended meaning of a word, pure from its other irrelevant meanings. Swapping word embeddings with sense embeddings requires the system to carry out an additional step: a word sense disambiguation module has to identify the intended meaning of ambiguous words (e.g., “cell”). Having identified the intended sense, the system can swap the word embedding with the corresponding sense embedding. This swapping coupled with the disambiguation stage can be regarded as a way of contextualizing each word’s representation to the semantics of its surrounding words.

However, there are multiple factors that limit the efficacy of sense embeddings. Firstly, word sense disambiguation is far from being optimal; hence, the initial stage of mapping words to word senses introduces inevitable noise to the pipeline [Pilehvar et al., 2017]. Secondly, it is not straightforward to benefit from raw texts, which are available at scale, to directly improve these representations. Hence, their coverage and semantic depth is limited to the knowledge encoded in lexical resources, which can be too restrictive. Thirdly, these representations are still not fully contextualized. The intended sense of a word in a given context is assumed to fully align with that defined in the target inventory, which might not be always true. For instance, the closest meaning for the noun “tweet” in WordNet is “a weak chirping sound as of a small bird” which certainly will not fully align if the intended meaning refers to “a post on Twitter”. Even worse, the intended meaning of the word, or the word itself, might not have been covered in the underlying sense inventory (for instance, the noun “embedding”, as it is widely used in NLP, is not defined in WordNet).

Unsupervised sense representations can be adapted to specific text domains; hence, they might not suffer as much in terms of coverage. However, they still need a disambiguation stage which is not be as straightforward as that for knowledge-based counterparts. Given that these representations are often produced as a result of clustering, their semantic distinctions are unclear and their mapping to well-defined concepts is not simple. Hence, a more complicated word sense disambiguation stage would be required, one that can disambiguate the input words according to the inventory of induced senses. Given that such a technique cannot easily benefit from rich sense-specific information available in existing lexical resources, it is usually not that effective. In fact, one of the main limitations of unsupervised sense representation models lies in their difficult integration into downstream models [Li and Jurafsky, 2015].

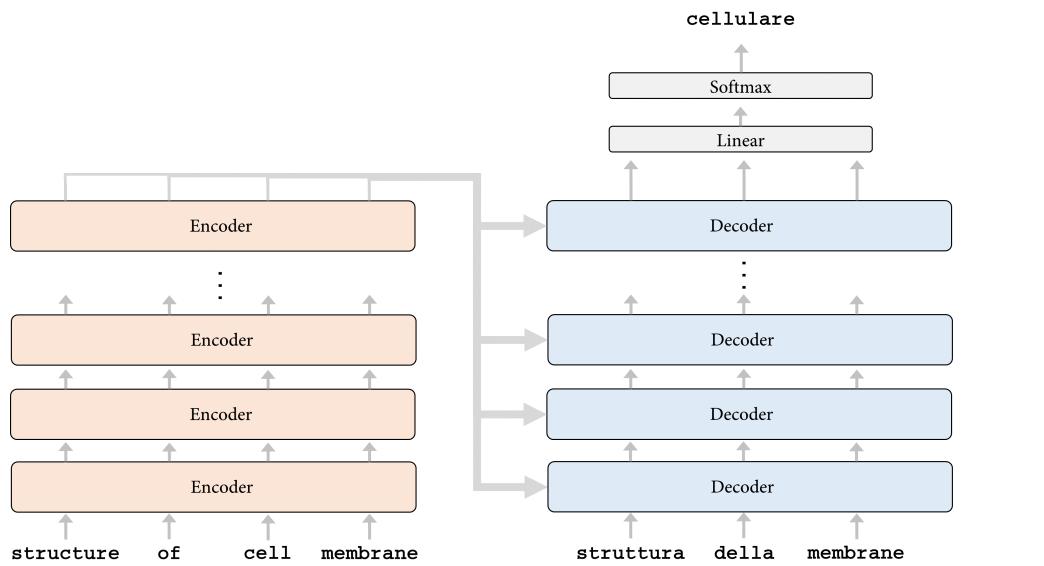


Figure 6.2: A high-level illustration of the Transformer model used for translation. The model is auto-regressive and has an encoder-decoder structure. The encoder and decoder have six identical encoders and decoders, respectively (only four shown here).

6.2 BACKGROUND: TRANSFORMER MODEL

Given that most of the recent literature on contextualized embeddings are based on a novel model called Transformer, in this section, we provide a brief overview of the Transformer architecture. Figure 6.2 provides a high-level illustration of the Transformer model. The model is an auto-regressive sequence transducer: the goal is to convert an input sequence to an output sequence, while the predictions are done one part at a time, consuming the previously generated parts as additional input. Similarly to most other sequence to sequence (Seq2Seq) models (cf. Section 2.2.2), the Transformer employs an encoder-decoder structure. However, unlike previous models which conventionally used a recurrent network (e.g., LSTM) for their encoder and decoder, the Transformer model is based on self-attention only with no recurrence. The Transformer forgoes the recurrence of RNN's for a fully feedforward attention-based architecture.

The main idea behind the Transformer model is self-attention. Self-attention, also known as intra-attention, is a mechanism that enables the sequence encoder to “attend” to specific parts of the sequence while processing a specific word.

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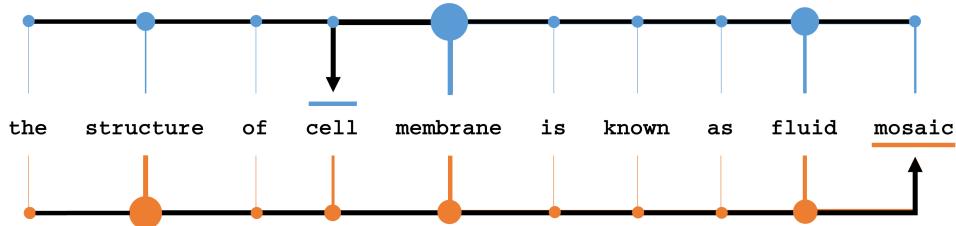


Figure 6.3: An illustration of self attention for the words *cell* (top) and *mosaic* (bottom). By attending to the context, particularly *membrane*, the interpretation of *cell* gets adapted to this specific usage and for the biological meaning. The same applies for *mosaic*, with a self attention mostly towards *structure*, *membrane*, and *fluid*. In the Transformer model, there are multiple spaces for self-attention (multi-head attention) that allows the model to have different interpretations in multiple representation sub-spaces.

6.2.1 SELF-ATTENTION

We saw in Section 2.2.2 the intuition behind the attention mechanism in sequence tranduction models. The basic idea was to focus the attention of the model to those source tokens for which the decoder is currently trying to generate the corresponding output (for instance, translation). The same idea can be applied to the process of reading and understanding of natural language text.

Figure 6.3 shows an example for self-attention for two semantically ambiguous words, *mosaic* and *cell*. Consider the word *cell*. Even for a human reading this sentence, it would be almost impossible to identify the intended meaning of the word unless the succeeding word (i.e., *membrane*) is taken into account. In fact, to be able to get a clear grasp of the meaning of a sentence, humans often require to scan the context or finish reading the sentence.

Self-attention, also known as intra-attention, is a special attention mechanism that tries to mimic this process. Instead of relating positions across two different sequences, self-attention looks for relations between positions in the same sequence. The goal of self-attention is to allow the model to consider the context while “reading” a word. For the case of our example, while “reading” the target word *cell* the self-attention mechanism focuses the attention to the word *membrane* in order to allow a better representation for the target word, adapted to the biological meaning. Note that, similarly to the Seq2Seq attention mechanism, self-attention is a *soft* measure: multiple words can be attended with varying degrees.

Consider the input sequence x_1, \dots, x_n . The self-attention mechanism maps the input embeddings for this sequence to an adapted output sequence z_1, \dots, z_n . For an

input word² x_t , the process of computing the self-attention vector z_t in the Transformer model can be summarized as follows:

1. For every input x_i , compute three different vectors: query q_i , key k_i , and value v_i . This is done by multiplying the input vector x_i with the corresponding matrices W^q , W^k , and W^v . The weights of these matrices are among the parameters that are learned during training.
2. Compute a score s_i for every input x_i . The score is computed as the dot product of the query vector q_t and the corresponding key vectors for every x_i (i.e., all k_i).
3. Normalize the scores by $\sqrt{d_k}$, where d_k is the dimensionality of the key (and query) vector.
4. Compute a weighted average of all value vectors (v_i), weighted by their corresponding scores s_i . The resulting vector is z_t .

The above procedure can be written as the following equation in matrix form:

$$\text{Attention}(Q, K, V) = \text{softmax}\left(\frac{QK^T}{\sqrt{d_k}}\right)V \quad (6.1)$$

The Transformer model makes use of multiple attention *heads*. In other words, multiple sets of W matrices are considered to produce different query, key, and value vectors for the same word. This allows the model to have multiple representation sub-spaces to focus on different positions.

6.2.2 ENCODER

The original Transformer model makes use of six identical encoder layers. Figure 6.4 (left) shows the stack of three of these encoders (for one, we are showing more details of the internal structure). Each encoder layer has two sub-layers: self-attention and feedforward. We saw in the previous section how the self-attention layer can help the model to look at the context words while “reading”, in order to get a clearer understanding of the semantics of individual tokens, and in turn the meaning of the sentence. As was explained before, each attention layer is coupled with multiple “heads”, with the hope of enabling the model to attend to different parts and two have multiple independent representation subspaces for capturing distinct patterns.

²In the actual model each word might be split into multiple tokens; for instance, *membrane* can be split into *mem*, *bra*, and *ne_*. The input to the model would be a sequence of tokens (rather than words).

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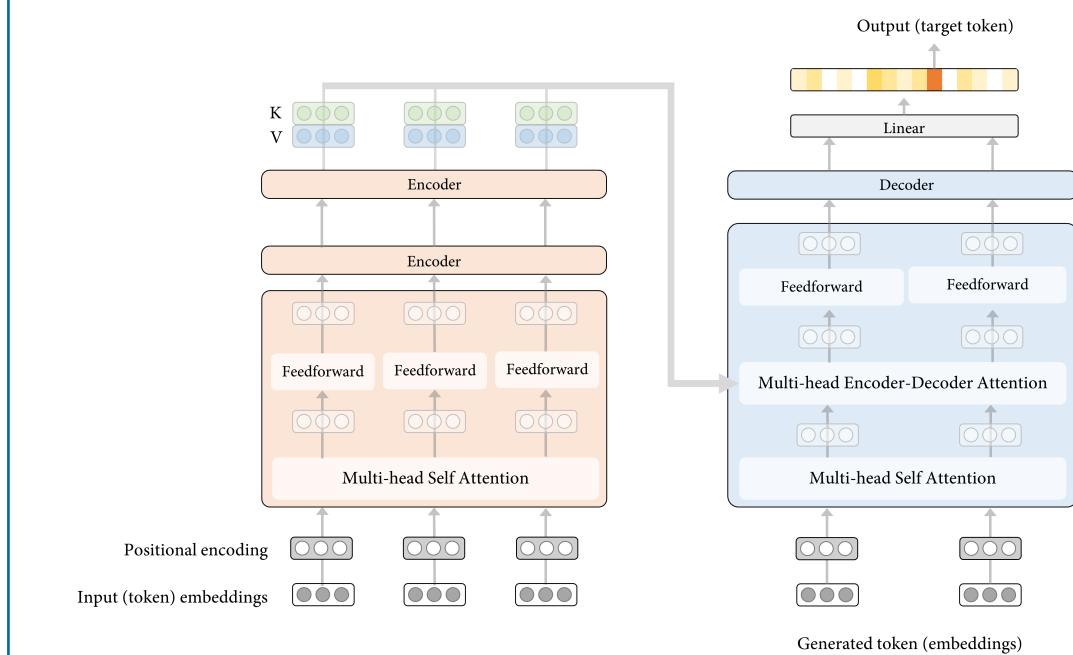


Figure 6.4: Encoders and decoders have similar internal structure, other than an encoder-decoder attention sub-layer added to the decoder. Input word embeddings are summed up with positional encodings and are fed to the bottom encoder. Decoders receive the outputs generated so far (as well as signal from the encoder) and predict the next token. Prediction is done via a fully-connected layer that generates the scores over the vocabulary (logits vector), followed by a softmax (to make the scores probability-like).

The z_i outputs of the self-attention sub-layer are fed to the feedforward sub-layer which is in fact a fully-connected network. The feedforward layer is *point-wise*, i.e., the same feedforward network is applied independently to individual z_i vectors.

6.2.3 DECODER

Similarly to the encoder, the decoder of the Transformer model also consists of a stack of six identical decoder layers. Each decoder is very similar to encoder in architecture with the slight difference that it has a third sub-layer which performs a cross-attention between encoder's output and decoder's state.³ Also, it is necessary

³Both decoder and encoder involve other small architectural details, such as residual connections around sub-layers and normalization. We skip these for simplicity.

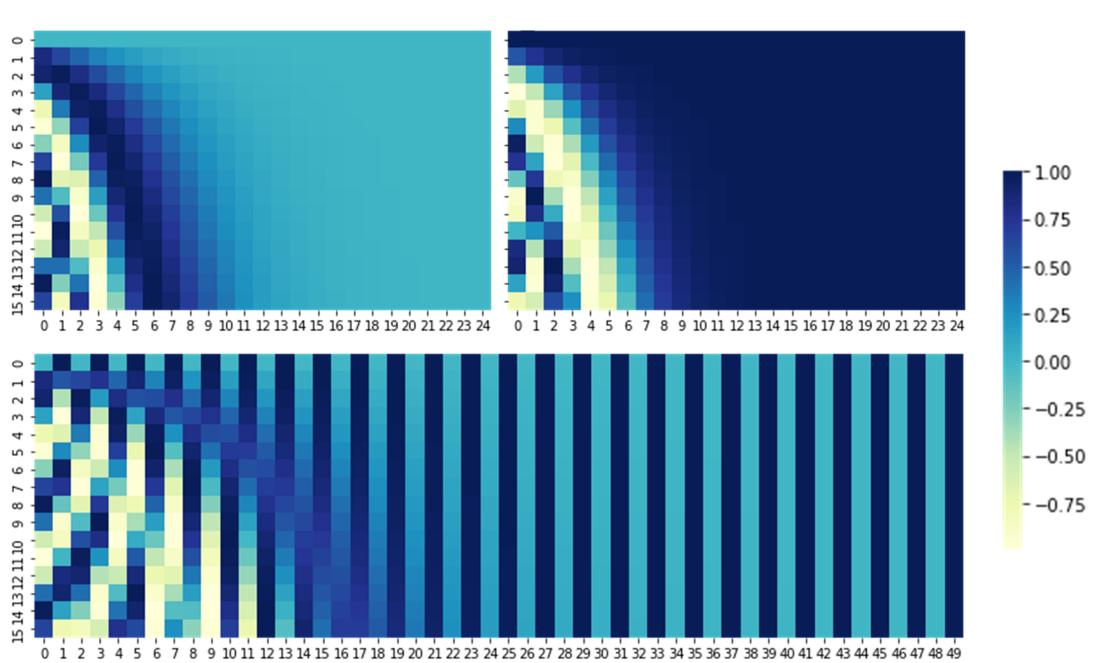


Figure 6.5: The positional encodings used to capture relative positions in the Transformer model. Sixteen encodings are visualised (rows), enough to encode a sequence of 16 tokens (10,000 in the original model). The model also uses 512- d encodings; but, for simplicity we show 50- d . Two sub-encodings are generated using $\sin()$ (top, left) and $\cos()$ (top, right) functions. The two are merged to generate the full encoding, shown at the bottom.

to modify the self-attention sub-layer in the decoder in order to prevent the model from attending to subsequent positions. Transformer achieves this by means of masking the subsequent positions. This masking is to ensure that the predictions at any position can depend only on the outputs generated so far (and not future outputs).

6.2.4 POSITIONAL ENCODING

As explained above, the Transformer model does not involve any recurrence (or convolution) to capture the relative positioning of tokens in the sequence. However, we know that word order is crucial to semantics; ignoring this would diminish the model to a simple bag-of-words. The authors of the Transformer model made use of a mechanism called positional encoding in order to inject information about token positions and hence making the model sensitive to word order.

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To this end, each input embedding to the encoder and decoder is added with a positional embedding which denotes the position of each input word with respect to the sequence. To facilitate the summation, positional encodings are of the same size as the input token embeddings. There can be different ways of encoding the position; Transformer makes use of a sinusoidal function. Specifically, the positional encoding P for the t^{th} token (starting from 0) is computed as follows:

$$\begin{aligned} D_i &= \frac{1}{10000^{\frac{2i}{d}}} \\ P(t, 2i) &= \sin(tD_i) \\ P(t, 2i + 1) &= \cos(tD_i) \end{aligned} \tag{6.2}$$

where $i \in \{0, \dots, d - 1\}$ is the encoding index, and d is the dimensionality of the positional encodings which is the same as input token embedding size (512 in the original model). An example is shown in Figure 6.5. Note that the final encoding is a merger of the two sub-encodings from $\sin()$ and $\cos()$ functions, where the former fills the even positions and the latter the odd ones.

6.3 CONTEXTUALIZED WORD EMBEDDINGS

Unlike static word embeddings, contextualized embeddings are representations of words in context. They can circumvent many of the limitations associated with word and sense embeddings, bringing about multiple advantages, one of the most important of which is seamless integration into most neural language processing models. Unlike knowledge-based sense representations, these embeddings do not rely on annotated data or external lexical resources and can be learned in an unsupervised manner. More importantly, their introduction to neural models does not require extra efforts such as word sense disambiguation as they function at the level of words. Interestingly, contextualized embeddings not only can capture various semantic roles of a word, but also its syntactic properties [Hewitt and Manning, 2019, Goldberg, 2019].

In contrast to static word embeddings which are fixed, contextualized word embeddings are *dynamic* in that the same word can be assigned different embeddings if it appears in different contexts. Therefore, unlike static word embeddings, contextualized embeddings are assigned to tokens as opposed to types. Instead of receiving words as distinct units and providing independent word embeddings for each, contextualized models receive the whole text span (the target word along with its context) and provide specialized embeddings for individual words which are adjusted to their context. Figure 6.6 provides an illustration: to produce a dynamic embedding for the target word (i.e., *cell*) the contextualized model analyzes the whole context.

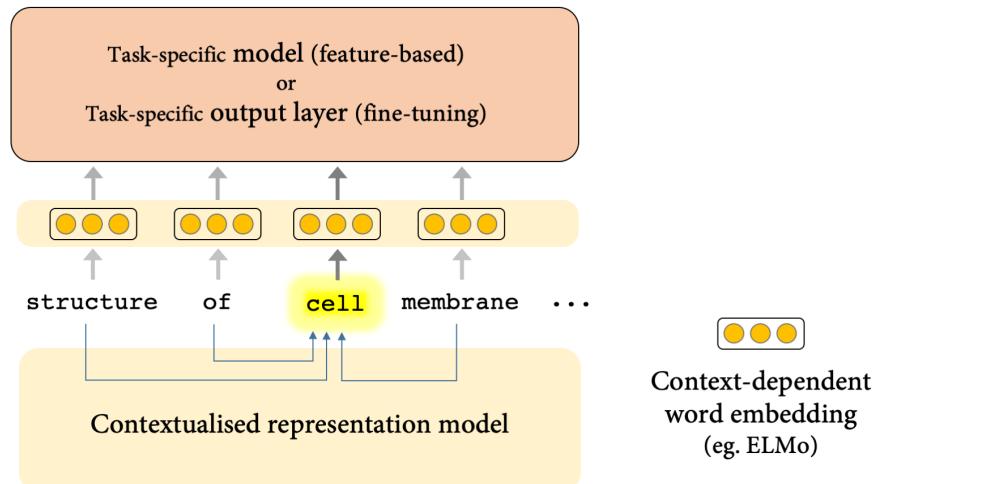


Figure 6.6: Unlike static (context-independent) word embeddings, contextualized (dynamic) embeddings are not fixed: they adapt to their representation to the context. The contextualized representation model processes the context of the target word (*cell* in the figure) and generates its dynamic embedding.

The following sections will provide more information on the specifics of the model in the figure.

6.3.1 EARLIER METHODS

The sequence tagger of [Li and McCallum \[2005\]](#) is one of the pioneering works that employ contextualized representations. The model infers context sensitive latent variables for each word based on a soft word clustering and integrates them, as additional features, to a CRF sequence tagger. The clustering technique enabled them to associate the same word with different features in different contexts.

With the introduction of word embeddings [[Collobert et al., 2011](#), [Mikolov et al., 2013c](#)] and the efficacy of neural networks, and in the light of meaning conflation deficiency of word embeddings, context-sensitive models have once again garnered research attention. **Context2vec** [[Melamud et al., 2016](#)] is one of the first proposals in the new branch of contextualized representations. Context2vec's initial goal was to compute a better representations for the context of a given target word. The widely-practised and usually competitive baseline to compute representation for multiple words (a piece of text) is to simply average the embedding of the words. This baseline is unable to capture important properties of natural language, such as word order or semantic prominence. Instead, Context2vec makes use of a

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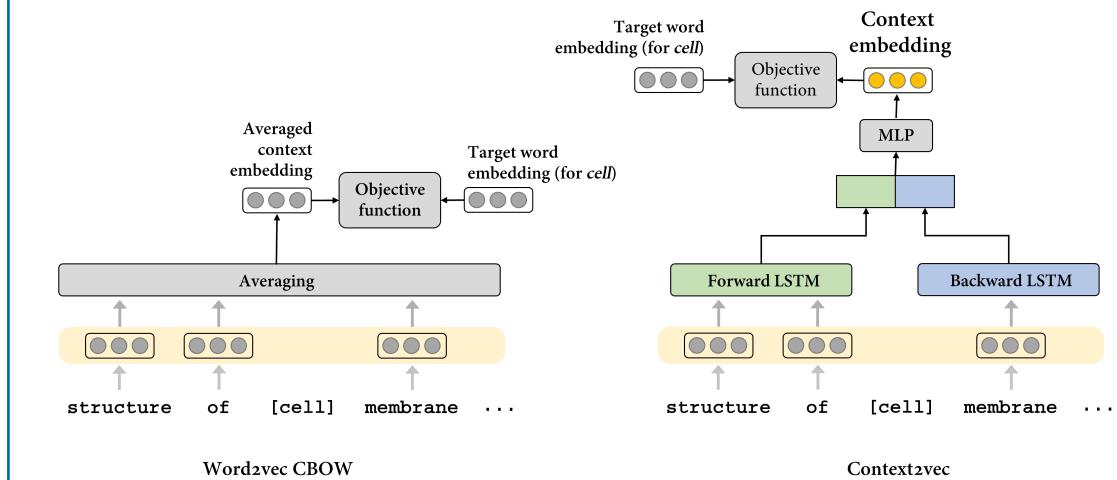


Figure 6.7: Architecture of Context2vec and how it differs from Word2vec CBOW: instead of modeling the context by naively averaging embeddings of words in the context window (as in CBOW), context2vec models the context using a bidirectional LSTM.

bidirectional LSTM language model to better encode these properties. Figure 6.7 shows the architecture of Context2vec and illustrates the different context modeling of this technique in comparison with Word2vec CBOW. Context2vec embeds sentential contexts and target words in the same semantic space.

The encoded representation for the context of a target word can be taken as the embedding of that word which is *contextualized* to its context. Hence, though the authors of Context2vec did not explicitly view the approach as a means of computing dynamic word embeddings, it is highly similar to subsequent works in contextualized word embeddings and constitutes one of the bases for this field of research. The most important distinguishing factor to subsequent techniques is that Context2vec ignores the target word while computing the contextualized representation, which turns out to be crucial.

6.3.2 LANGUAGE MODELS FOR WORD REPRESENTATION

As was discussed in Chapter 2, Language Models (LM) aim at predicting the next word in a sentence given the preceding words. To be able to accurately predict a word in a sequence, LMs need to encode both the semantic and syntactic roles of words in context. This makes them suitable candidates for word representation. In fact, nowadays, LMs are key components not only in natural language generation, but also

in natural language understanding. Additionally, knowledge acquisition bottleneck is not an issue for LMs, since they can essentially be trained on multitude of raw texts in an unsupervised manner. In fact, extensive models can be trained with LM objectives and then transferred to specific tasks. Though still at early stages, this technique has been shown to be a promising direction [Radford et al., 2018], reminiscent of the pre-training procedure in Computer Vision which involves training an initial model on ImageNet or other large image datasets and then transferring the knowledge to new tasks.

Figure 6.6 provides a high-level illustration of the integration of contextualized word embeddings into an NLP model. At the training time, for each word (e.g., *cell* in the figure) in a given input text, the language model unit is responsible for analyzing the context (usually using sequence-based neural networks) and adjusting the target word’s representation by contextualising (adapting) it to the context. These context-sensitive embeddings are in fact the internal states of a deep neural network which is trained with language modeling objectives either in an *unsupervised* manner [Peters et al., 2017, Peters et al., 2018] or on a *supervised* task, such as bilingual translation configuration [McCann et al., 2017]. The training of contextualized embeddings is carried out as a pre-training stage, independently from the main task on a large unlabeled or differently-labeled text corpus. Depending on the sequence encoder used in language modeling, these models can be put into two broad categories: **RNN** (mostly LSTM) and **Transformer**.

6.3.3 RNN-BASED MODELS

For this branch of techniques, the “Contextualized representation model” in Figure 6.6 is on the shoulders of an LSTM-based encoder, usually a multi-layer bidirectional LSTM (BiLSTM). LSTMs are known to be able to capture word order to some good extend. Also, unlike the word embedding averaging baseline, LSTMs are capable of combining word representations in a more reasonable manner, giving higher weights to those words that are semantically more central in the context. The TagLM model of Peters et al. [2017] is a an example of this branch which trains a BiLSTM sequence encoder on monolingual texts. The outputs of the sequence encoder are concatenated and fed to a neural CRF sequence tagger as additional features.

The Context Vectors (CoVe) model of McCann et al. [2017] similarly computes contextualized representations using a two-layer biLSTM network, but in the machine translation setting. CoVe vectors are pre-trained using an LSTM encoder from an attentional sequence-to-sequence machine translation model.⁴

⁴In general, the pre-training property of contextualized embeddings makes them closely related to transfer learning [Pratt, 1993], which is out of the scope of this book. For more detailed information on transfer learning for NLP, we would refer to [Ruder, 2019].

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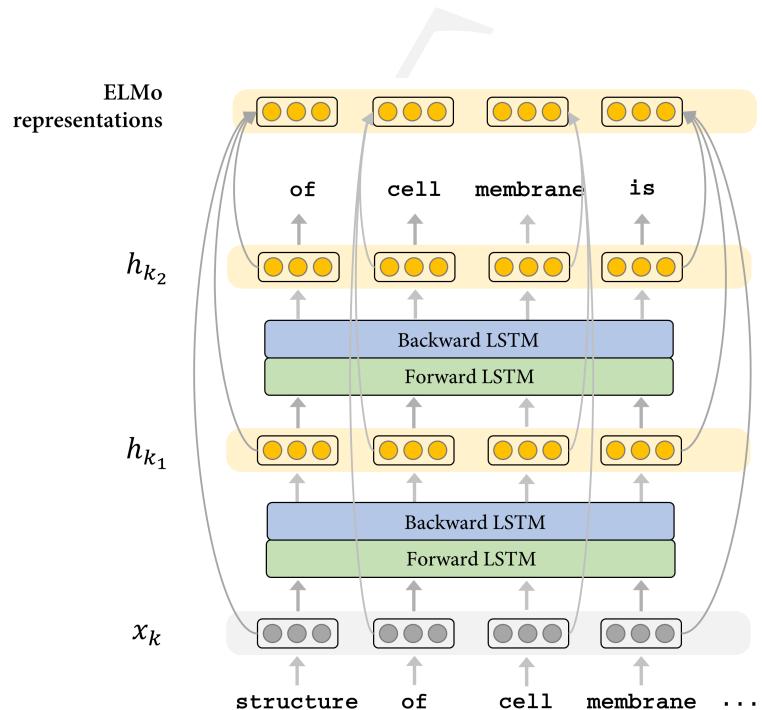


Figure 6.8: ELMo makes use of a 2-layer bidirectional LSTM to encode words in the context word. The ELMo representation for the target word is a combination of the hidden states of the two BiLSTM layers, i.e., h_{k_1} and h_{k_2} , which encode the context-sensitive representation of each word, and the static representation of the word, i.e., x_k , which is character-based. ELMo uses some residual connections across LSTMs which are not shown in the figure for simplicity.

The prominent **ELMo** (Embeddings from Language Models) technique [Peters et al., 2018] is similar in principle. A multi-layer (two in the original model) BiLSTM sequence encoder is responsible for capturing the semantics of the context. The main difference between TagLM and ELMo lies in the fact that in the latter some weights are shared between the two directions of the language modeling unit. Figure 6.8 provides a high-level illustration of how ELMo embeddings are constructed. A residual connection between the LSTM layers allows the deeper layer(s) to have a better look at the original input and to allow the gradients to better backpropagate to the initial layers. The model is trained on large amounts of texts with the language modeling objective: given a sequence of tokens, predict the next token. The trained model is then used to derive contextualized embeddings that can be used as input into various NLP systems.

There can be multiple ways for combining the outputs of ELMo model, i.e., the hidden states of the two BiLSTM layers, h_{k_1} and h_{k_2} , and the context-independent representation x_k . One may take only the top layer output or concatenate the three layers to have long vectors for each token, to be fed as inputs to an NLP system. One can also learn a weighted combination of the three layers, based on the target task, or concatenate other static word embeddings with ELMo embeddings. ELMo makes use of character-based technique (based on Convolution Neural Networks) for computing x_k embeddings. Therefore, it benefits from all the characteristics of character-based representations (cf. Section 3.3), such as robustness to unseen words.

6.4 TRANSFORMER-BASED MODELS: BERT

The introduction of **Transformers** [Vaswani et al., 2017] and their immense potential in encoding text sequences resulted in another boost in the already fast-moving field of LM-based contextualized representations. Transformers come with multiple advantages over recurrent neural networks (which were previously the dominant role players): (1) compared to RNNs which process the input sequentially, Transformers are parallel which makes them suitable for GPUs and TPUs which excel at massive parallel computation; (2) Unlike RNNs which have memory limitation and tend to process the input in one direction, thanks to the self-attention mechanism (cf. Section 6.2.1), Transformers can attend to contexts about a word from distant parts of a sentence, both earlier and later than the word appears, in order to enable a better understanding of the target word without any locality bias. For instance, the word “cell” in Figure 6.8 can be disambiguated by looking at the next word in the context, “membrane”.

The impressive initial results obtained by Transformers on sequence to sequence tasks, such as Machine Translation and syntactic parsing [Kitaev and Klein, 2018], suggested a potential replacement for LSTMs in sequence encoding tasks. As

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of now, Transformers are dominantly exceeding the performance levels of conventional recurrent models on most NLP tasks that involve sequence encoding.

The OpenAI's **GPT** model (Generative Pre-trained Transformer) [Radford, 2018] was one of the first attempts at representation learning using Transformers. Moving from LSTMs to Transformers resulted in a significant performance improvement and enabled a more effective way of fine-tuning the pre-trained models to specific tasks.

The architecture of the Transformer model was discussed in Section 6.2. The GPT model is based on a modified version of Transformer, called the Transformer Decoder [Li et al., 2018], which discards the encoder part. Therefore, instead of having a source and a target sentence for the sequence transduction model, a single sentence is given to the decoder. Instead of generating a target sequence, the objective is set as a standard language modeling in which the goal is to predict the next word given a sequence of words. GPT was also one of the first works to popularize the fine-tuning procedure (to be discussed in Section 6.6).

However, like ELMo, GPT was based on unidirectional language modeling. While reading a token, GPT can only attend to previously seen tokens in the self-attention layers. This can be very limiting for encoding sentences, since understanding a word might require processing future words in the sentence. This is despite the fact that Transformers are characterized by their self-attention layer and the capability of receiving the input sequence in parallel. What hindered a bidirectional Transformers was that bidirectional conditioning would result in a word to indirectly "see" itself in a multi-layered context.

BERT. BERT, short for Bidirectional Encoder Representations from Transformers [Devlin et al., 2019] revolutionized the NLP field in 2018/2019. Similarly to GPT, BERT is based on the Transformer architecture; however, BERT makes use of the full encoder-decoder architecture (see 6.2 for more details).

The essential improvement over GPT is that BERT provides a solution for making Transformers bidirectional. This addition enables BERT to perform a joint conditioning on both left and right context in all layers. This is achieved by changing the conventional next-word prediction objective of language modeling to a modified version, called Masked Language Modeling.

6.4.1 MASKED LANGUAGE MODELING

Before BERT, the commonly-practised language modeling objective was to predict the next token (given a sequence of tokens). Inspired by the cloze test [Taylor, 1953], BERT introduced an alternative language modeling objective to be used during the training of the model. According to this objective, instead of predicting the next to-

ken, the model is expected to guess a “maseked” token; hence, the name Masked Language Modeling (MLM). MLM randomly masks some of the tokens from the input sequence (15% for example), by replacing them with a special token, e.g., “[MASK]”.

For instance, the sequence “the structure of cell membrane is known as fluid mosaic” is changed to “the structure of cell [MASK] is known [MASK] fluid mosaic”. The goal would be to predict the masked (missing) tokens based on the information available from unmasked tokens in the sequence. This allows the model to have conditioning not only on the right (next token prediction) or left side (previous token prediction), but on context from both sides of the token to be predicted.

To be more precise, given that the [MASK] token only appears during the training phase, BERT employs a more comprehensive masking strategy. Instead of always replacing the token with the special [MASK] token (that has 80% chance), BERT sometimes replaces the word with a random word (10% chance) or with the same word (10%).

It is important to note that the model is not provided with the information on missing words (or words that have been replaced). The only information is the proportion of this change (e.g., 15% of the input size). It is on the model to guess these words and suggest predictions/replacements. The objective enabled BERT to capture both left and the right contexts, and to alleviate the unidirectional limitation of earlier models.

6.4.2 NEXT SENTENCE PREDICTION

In addition to the MLM objective, BERT also uses a Next Sentence Prediction (NSP) task in which the model has to identify if a given sentence can be considered as the subsequent sentence to the current sentence or not. This is motivated by the fact that to perform good in some tasks the model needs to encode relationships between sentences or to resort to information that are beyond the boundary of the sentence.

The task is a binary classification. For each sentence A the mode is provided with a second sentence B and is asked if B is the next sentence for A ? To make a balanced self-training dataset, the actual next sentence is replaced with a random sentence 50% of the time. This objective helps the model in learning the relationships between sentences and was shown to be beneficial in tasks such as Natural Language Inference and Question Answering [Devlin et al., 2019].

6.4.3 TRAINING

The training objective of BERT is to minimize a combined loss function of MLM and NSP. Note that the training of BERT is carried out on pairs of sentences (given the NSP objective). In order to distinguish the two input sentences, BERT makes use of two special tokens: [CLS] and [SEP]. The [CLS] token is inserted at the beginning

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and the [SEP] token in between the two sentences. The entire sequence is then fed to the encoder. The output of the [CLS] token encodes the information about the NSP objective and is used in a softmax layer for this classification.

The original BERT is trained in two settings: Base and Large. The two versions differ in their number of encoder layers, representation size and number of attention heads. BERT has given rise to several subsequent models, many of which are in fact variations of the original BERT in terms of the training objective or the number of parameters.

Subword tokenization. Unlike conventional word embedding techniques, such as Word2vec and GloVe, that take whole words as individual tokens and generate an embedding for each token, usually resulting in hundreds of thousand or millions of token embeddings, more recent models, such as BERT and GPT, segment words into subword tokens and aim at embedding these units. In practise, different tokenization algorithms are used in order to split words into subword units.

Segmenting words into subword units can bring about multiple advantages: (1) It drastically reduces the vocabulary size, from millions of tokens to dozens of thousands; (2) It provides a solution for handling out-of-vocabulary words as any unseen word can theoretically be re-constructed based on its subwords (for which embeddings are available); (3) It allows the model to share knowledge among words that have similar structures (look similar) with the hope that they share semantics, for instance, cognates across different languages or lexically-related terms in the same language.

The most commonly used tokenizers are Byte-Pair Encoding (BPE) and WordPiece tokenizer. Both tokenizers leverage a similar iterative algorithm: the vocabulary is initialized with all the characters (symbols) in a given text corpus. Then in each iteration, the vocabulary is updated with the most likely pairs of existing symbols in the vocabulary. BPE [Witten et al., 1994] takes the most frequent pair as the most “likely” one whereas WordPiece [Schuster and Nakajima, 2012] considers likelihood on the training data.

6.5 EXTENSIONS

BERT is undoubtedly a revolutionary proposal that has changed the landscape of NLP. Therefore, it is natural to expect massive waves of research on improving the model or on applying the ideas from the model or the model itself to various other tasks in NLP.

Many of the extensions to BERT mainly rely on changing hyperparameters, either increasing the amount of training data or model capacity, with the hope of pushing the performance barriers on various benchmarks. For instance, **RoBERTa** [Liu et al., 2019b] removes BERT’s next-sentence pretraining objective which was shown to be non-optimal. RoBERTa trains with much larger mini-batches and learning rates on an order of magnitude more data than BERT, and for longer sequences of input. This all results in a boost in BERT’s performance, for instance, around 15% in the SuperGLUE benchmark.

It is important to note that the recent trend has been to pre-train larger and larger⁵ models on bigger datasets to investigate the limits of transfer learning [Raffel et al., 2019]. However, not all extensions to BERT can be reduced to sole modifications of hyperparameters or to pushing model size. In the following sections, we will briefly overview some of the limitations of BERT and how different extensions have tried to address these.

6.5.1 TRANSLATION LANGUAGE MODELING

XLM [Lample and Conneau, 2019] modifies the training objective of BERT to achieve a better multi-lingual model. XLM introduces a cross-lingual training objective. Similarly to BERT, the objective is to predict the masked token but in the case of XLNet the model is asked to use the context from one language to predict tokens in another language. This multi-lingual objective was shown to result in representations that are significantly better than BERT in tasks that require cross-lingual transfer of knowledge obtained during training from one language to another, to allow zero-shot application in an unseen language.

Moreover, XLM makes use of Byte-Pair Encoding (BPE), instead of working on word and tokens. BPE splits the tokens into the most common sub-tokens across all languages, allowing XLM to have a larger shared vocabulary between languages.

6.5.2 CONTEXT FRAGMENTATION

Dai et al. [2019] point out an issue with the Transformer architectures. The limitation, which they refer to as *context fragmentation*, is the result of inputting fixed length text segments to models such as BERT. These segments are usually fixed in size and do not take into account sentence boundary or any other semantic criteria. Therefore, the model cannot learn long-term dependencies that do not fit within the pre-defined context. In addition, there is no information flow across segments in these models. This leaves the model with no contextual information to predict the first few tokens.

⁵For instance, Megatron-LM (NVidia) and Turing-NLG (Microsoft Research) push the 340M parameters of BERT-large to the astronomical 8B and 17B parameteres, respectively.

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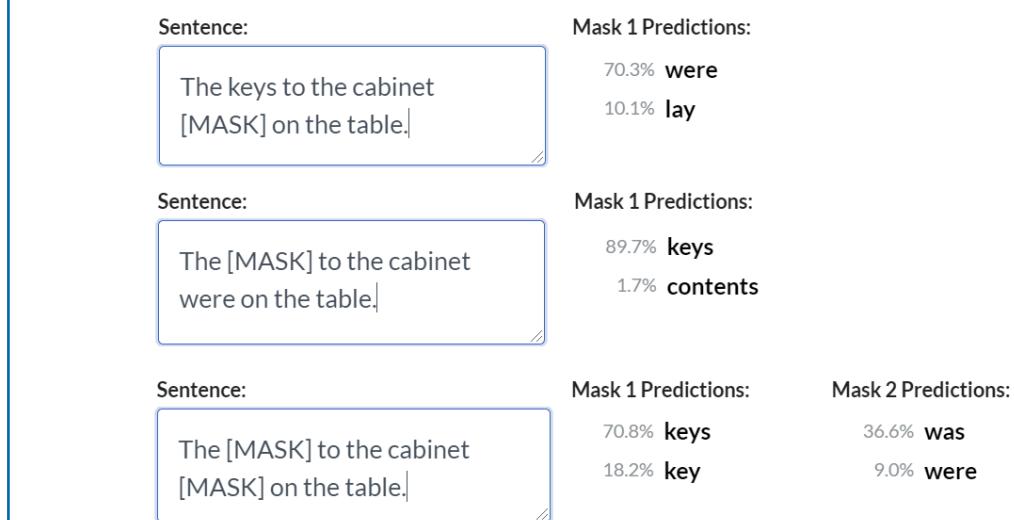


Figure 6.9: The parallel independent prediction in Masked Language Modeling of BERT prevents the model from taking into account dependencies between masked words which are to be predicted. Screenshot from AllenNLP’s BERT MLM demo⁶.

Dai et al. [2019] proposed a model, called **Transformer-XL** (extra long), which allows the Transformer architecture to learn long-term dependencies across segments, hence addressing the segment fragmentation issue. This is achieved by adding a recurrence across segments, i.e., consecutive sequences of computation. This way, at any computation, the model is provided with information from the previous segments which can be used for both generating the starting tokens, and to allow the model to look for dependencies that go beyond segment boundaries.

In order to give a “temporal clue” to the model to distinguish among positions in different segments, they also had to upgrade the positional encoding mechanism. The positional encoding, as explained in Section 6.2.4 is unable to distinguish the positional difference between tokens in different segments at different layers. Therefore, Dai et al. [2019] also put forward the *relative* positional encoding in order to make the recurrence mechanism of the model to avoid temporal confusion.

6.5.3 PERMUTATION LANGUAGE MODELING

As was mentioned in Section 6.2, the original Transformer model is autoregressive: the generated outputs until timestep t will be used as additional input to generate the $t + 1^{th}$ output. BERT proposes an autoencoder model based on the MLM objective

(Section 6.4.1) which allows the language model to be conditioned on both directions (“see” context from both sides of the word to predict).

Despite the desirable property of enabling the model to see “future” context, autoencoder models have their own disadvantages. Importantly, BERT uses the [MASK] symbol in the pretraining, but this artificial symbols are absent from the real data at finetuning time, resulting in a *pretrain-finetune discrepancy*. Another main disadvantage of BERT’s autoencoder model is that it assumes that the masked tokens can be predicted only based on the other given unmasked tokens, and independently from each other. This can be essentially incorrect as masked words constitute around 15% of the context; hence, taking into account the correlations among them can be crucial for accurate prediction. Figure 6.9 shows an example for cases that the independent assumption of MLM can cause syntactic discrepancies.

XLNet [Yang et al., 2019] addressed the pretrain-finetune discrepancy and parallel independent predictions of BERT’s MLM by proposing a new objective called *Permutation Language Modeling* (PLM). PLM is similar in objective to traditional language models: predict one token given context. However, instead of receiving the context in a sequential order, as is the case for traditional language models, PLM predicts tokens in a random order. In other words, the task in PLM is to predict a missing token in a sequence using any combination of other words in that sequence (irrespective of their position). This forces the PLM to model the more difficult task of learning the dependencies between all combinations of tokens in contrast to the traditional language models that only model dependencies in one direction.

XLNet is based on Transformer-XL architecture and benefits from the recurrence across segments. The main contribution is the PLM objective which provides a reformulation of language modeling. In order to make PLM work and to integrate it into the Transformer architecture, the authors had to address some other technical details (not discussed here), such as modifying the positional information through *Two-stream Self-attention*.

6.5.4 REDUCING MODEL SIZE

As was explained above, the general trend has been to push the models in size in order to investigate the limits of transformers in capturing complexities of natural language. However, a recent trend has started to move in the opposite direction: reducing model size while retaining the performance.

ALBERT [Lan et al., 2019] is one of the most recent Transformer-based models in this branch which provides some innovations that allow increasing the hidden layer size and the depth of the network without increasing the overall number of parameters. Other than changing the NSP objective of BERT for a Sentence-Order Prediction (SOP), which showed effective in multi-sentence encoding tasks, ALBERT

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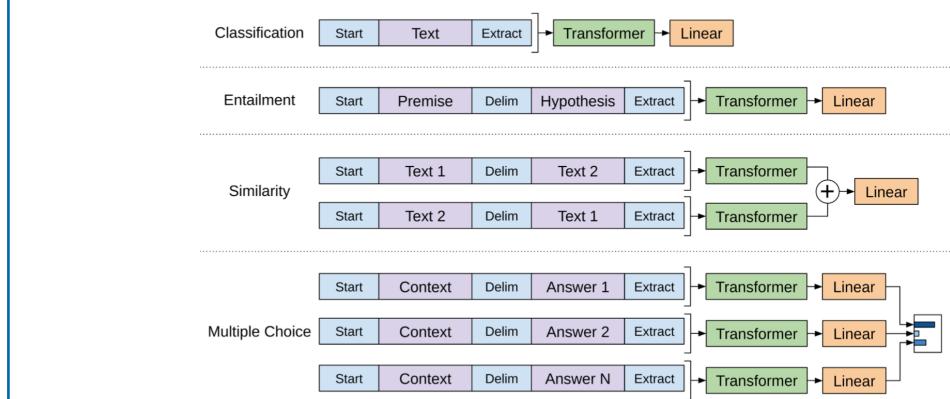


Figure 6.10: Fine-tuning of GPT to four different tasks. This setting involves minimal modifications to the pre-trained (language) model, usually in the form of changing the last layer, in to make them task specific (Image from [Radford \[2018\]](#)).

introduced two parameter reduction techniques to lower memory requirements and to speed up training. One is the cross-layer parameter sharing: the same set of parameters are used across layers. This prevents the number of parameters from growing along with the depth of the network, making the model significantly smaller in size. The other technique is to decompose the vocabulary matrix into two smaller matrices, which allows the hidden size to grow without significantly increasing the parameter size of the vocabulary embedding.

DistilBERT is another model in this trend that leverages knowledge distillation [[Bucila et al., 2006](#), [Hinton et al., 2015](#)] during the pre-training phase to construct lighter models that can perform competitively.

6.6 FEATURE EXTRACTION AND FINE-TUNING

One of the distinguishing features of recent pre-training work (such as GPT, BERT, and GPT-2) is to leverage the language model directly for the end task. Contextualized word embeddings can be utilized in two different ways:

Feature extraction. In this setting, the contextualized embeddings are fed as pre-trained *features* to a task-specific model. The model has a task-specific architecture (the weights of which are randomly initialized) and the embeddings are integrated as additional features to this model. This setting usually requires large amount of task-specific training data to be effective given that all weights of the main model need

to be trained from scratch. The contextualized model is used as a feature extractor which is able to encode semantic and syntactic information of the input into a vector.

Fine tuning. This approach, first popularised by GPT and ULMFiT [Howard and Ruder, 2018], gets closer to *one system for all tasks* setting. Fine-tuning mitigates the need for having task-specific models by transferring a pre-trained language model directly to a distant task through minimal modifications (usually in terms of changes in the last layer). This setting involves minimal modifications to the pre-trained model in order to make it suitable for the task.

Figure 6.10 shows an illustration of the fine-tuning used in GPT. All structured inputs are converted into token sequences which are input to the pre-trained model, followed by a shallow linear+softmax layer. [Peters et al., 2019] provides an experimental analysis of the two settings.

GPT-2 takes this setting to the extreme and alleviates the requirement for supervised learning on task-specific datasets (zero-shot task transfer). One interesting finding of the article is to show that reasonable results can be gained with no task specific fine tuning and by just framing the task as predicting conditional probabilities.

6.7 ANALYSIS AND EVALUATION

Contextualized models have shown great potential in a wide range of NLP applications, either semantic or syntactic. Moreover, the possibility to fine-tune and directly utilize these models in a diverse set of downstream NLP tasks suggests that they encode various sorts of syntactic and semantic knowledge.

In terms of semantics, despite the young age, BERT is now dominating top rows in many benchmarks, including GLUE [Wang et al., 2019b] and SuperGLUE⁷ [Wang et al., 2019a].

However, similarly to most other deep learning methods, the underlying procedure followed to achieve these cannot be unveiled unless some network analysis experiments are used to expose the hidden aspects, such as those analytical studies performed for visualising CNNs [Qin et al., 2018] or for understanding capabilities of LSTMs [Linzen et al., 2016, Gulordava et al., 2018].

In this line, many researchers have proposed “probe” experiments to explain the effectiveness of Transformer-based models on various NLP tasks. Probing usually involves checking if a linear model is able to correctly predict a linguistic property, syntactic or semantic, based on the representations. High performance in this

⁷For instance, on the Word-in-Context dataset [Pilehvar and Camacho-Collados, 2019], a simple binary classifier based on BERT, without any task-specific tuning, significantly improves all existing sense representation techniques which explicitly model various word senses.

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prediction is often taken as an evidence for the fact that the relevant information for the task is encoded in the representation.

Given that this is an active area of research with dozens of papers, sometimes with contradicting conclusions, it is not possible to cover all the relevant work. In the following, we briefly describe few of the more prominent works in this direction.

6.7.1 SELF ATTENTION PATTERNS

Self-attention is a key feature to Transformer-based models. Therefore, analyzing its behaviour, for instance in terms of the semantic or syntactic patterns they capture, constitutes an interesting research question, the answer to which would be crucial for understanding Transformer-based models and would allow us to better pursue possible paths towards improving the efficiency and capacity of these models.

[Clark et al. \[2019\]](#) carried out an experiment to check the attention distribution across attention heads. The findings suggested that heads within the same layer often have similar distributions, suggesting possible redundancy across attention patterns.

[Kovaleva et al. \[2019\]](#) further analyzed the the possibility of encoding redundant information by different attention heads. The general finding was that even the smaller pre-trained BERT model (i.e., *base*) is heavily overparametrized. The conclusion is based on the observation that there are many repeated self-attention patterns across different heads. This is also supported by the discovery that disabling some heads or even whole layers does not necessarily result in performance drop, but sometimes can lead to improvements. This observation corroborates the redundancy suggested by [Clark et al. \[2019\]](#) and is in line with the findings of [Michel et al. \[2019\]](#) and [Voita et al. \[2019\]](#) that a small subset of trained heads in each layer (sometimes a single one) might be enough at test time for preserving the same level of performance, in tasks such as translation.

[Kovaleva et al. \[2019\]](#) also investigated how the self-attention patterns change after fine-tuning of a pre-trained model. For most tasks in the GLUE benchmark, they concluded that it is the last one or two layers of the Transformer that encode most of the task-specific information during fine-tuning.

6.7.2 SYNTACTIC PROPERTIES

As for syntactic abilities, [Clark et al. \[2019\]](#) investigated the attention mechanism of BERT and found that certain attention heads encode to a high accuracy some syntax-sensitive phenomena, such as direct objects of verbs, determiners of nouns, objects of prepositions, and coreferent mentions. The subject-verb agreement was also investigated by [Goldberg \[2019\]](#). Specifically, it was shown that BERT assigns higher scores to the correct verb forms as opposed to the incorrect one in a masked language modeling task. This is despite the fact that, by design, Transformers do not

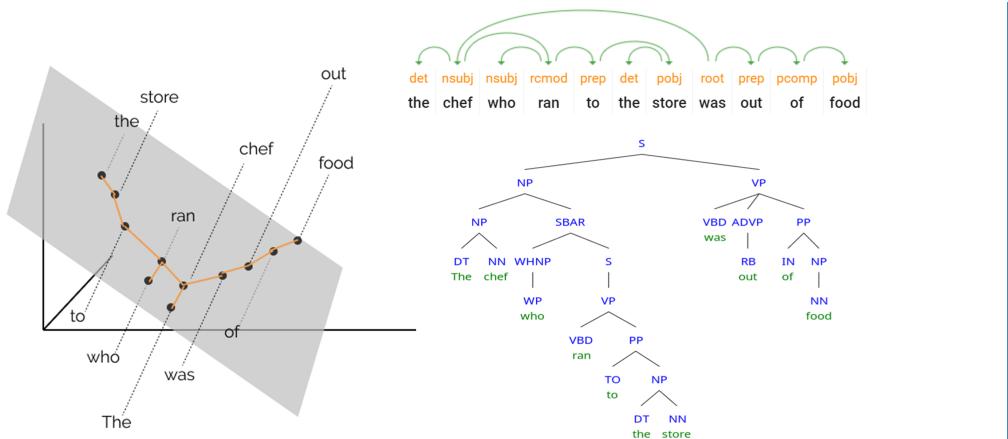


Figure 6.11: Hewitt and Manning [2019] showed that the minimum spanning tree over a linearly transformed space of contextualized embeddings (left) can estimate the dependency parse tree (top right) of a sentence or phrase to a good degree of accuracy. Illustration courtesy of the original work. The syntactic parse tree is generated using Stanford Parser and the dependency parse by Google NL API.

have an explicit means of capturing word order beyond a simple tagging of each word with its absolute-position embedding.

In the same spirit, Hewitt and Manning [2019] proposed a “probe” in order to investigate the extent to which contextualized models encode human-like parse trees. For this purpose, given a phrase or sentence, they learn a linear transformation to the contextualized embeddings of the words. Then, a minimum spanning tree is obtained for the transformed representations which is taken as the estimated parse tree. The results were surprising. The authors showed that the obtained tree matches the syntactic parse to a good extent.

The results clearly indicated that, even though the contextualized models are trained with a language modeling objective but they implicitly encode the syntax of the language since it might indirectly help them in fulfilling the objective. Linzen et al. [2016] provided an analysis on how capturing syntactic information can be crucial for accurate language modeling. The sentence in Figure 6.9 is from the same authors and clearly indicates an example for this.

Figure 6.11 shows an example for the sentence “the chef who ran to the store was out of food”. The minimum spanning tree estimated by the above procedure (shown on left) closely resembles the syntactic parse tree shown on the right.

In the contrary, Ettinger [2020] showed that BERT falls short of effectively encoding the meaning of *negation*, highlighted by a complete inability to prefer true

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over false completions for negative sentences. They also showed that, to a large extent, BERT is insensitive to malformed inputs as the predictions did not change when the input word order was shuffled or it was truncated. The same observation was made by [Wallace et al. \[2019\]](#), suggesting that BERT’s encoding of syntactic structure does not necessarily indicate that it actually relies on that knowledge.

6.7.3 DEPTH-WISE INFORMATION PROGRESSION

[Peters et al. \[2018\]](#) performed an empirical study to see how the choice of neural structure (LSTM, CNN, or Transformer) influences the accuracy of learned representations in different NLP tasks. Additionally, they showed that the learned representation differ in their properties at different depths of the network. Initial layers tend to encode only high-level morphological information, middle levels encode local syntactic properties, and top layers encode long-range semantic relations such as co-reference. Similar findings are reported by [Jawahar et al. \[2019\]](#) on a number of semantic and syntactic probing tasks and by [Raganato and Tiedemann \[2018\]](#) on the task of translation. Also, the prevalence of syntactic information in the middle layers is shown by other researchers, such as [Vig and Belinkov \[2019\]](#), [Liu et al. \[2019a\]](#) and [Tenney et al. \[2019\]](#).

[Lin et al. \[2019\]](#) further studied the the hierarchical organization of a sentence in BERT representations. They found that the hierarchical information increases in representations as we move to deeper layers, while the prevalence of linear/sequential information decreases. This suggests that in the deeper layers BERT replaces positional information for hierarchical features of increasing complexity.

[Tenney et al. \[2019\]](#) carried out another interesting analysis on the layers of BERT and showed that they resemble an NLP pipeline. Their analysis showed that the layers encode different tasks in a natural progression from basic syntactic information to high-level semantic information: part of speech tagging, followed by constituents, dependencies, semantic roles, and coreference. This gradual hierarchy of linguistic information from surface features to syntactic and then semantic features was also shown by [Jawahar et al. \[2019\]](#). [Tenney et al. \[2019\]](#) also showed that syntactic information tend to be concentrated on a few layers while semantic information is generally spread across the network.

6.7.4 MULTILINGUALITY

The authors of BERT have released a *multilingual* version trained on over 100 languages. The model is trained on monolingual corpora derived from Wikipedia for different languages, tokenized by the WordPiece tokenizer (cf. Section 6.4.3).

The model is shown to perform surprisingly good at zero-shot cross-lingual model transfer in which task-specific data in a (resource-rich) language is used in fine-

tuning for evaluation in other languages even with different scripts [Wu and Dredze, 2019]. The results are surprising given that the pre-training of multilingual BERT (M-BERT) does not involve any cross-lingual objective to encourage learning a unified multilingual representation. Moreover, M-BERT does not make use of aligned data, rather monolingual data in different languages.

One key question that can be asked with respect to multilinguality of M-BERT is the extent to which these representations resemble an interlingua, i.e., a common multilingual space in which semantically similar words across languages are placed in close proximities. Singh et al. [2019] is one of the first works that investigates this question. Using a set of probing experiments based on Canonical Correlation Analysis (CCA), they showed that the representations tend to partition across different language rather than sharing a common interlingual space. The partitioning effect was shown to get magnified in deeper layers, suggesting that the model does not progressively abstract semantic content while disregarding languages. They also showed that the choice of tokenizer for BERT can significantly influence the structure of the multilingual space the commonalities across representations in different languages, with the subword tokenizer having a strong bias towards the structure of phylogenetic tree of languages.

Another question that might arise is the impact of WordPiece tokenizer and the resulting subword overlap in the multilingual abilities of M-BERT. Is the effectiveness of M-BERT in zero-shot cross lingual transfer due to the vocabulary memorization of the model? Is the representational power of M-BERT transferrable across languages with no lexical overlap? Pires et al. [2019] provided an analysis on the same question. They opted for Named Entity Recognition (NER) as target task, given that entities are often similar across languages and hence a basic vocabulary memorization would allow the model to perform well across similar languages but fail for languages with small lexical overlap. They showed that M-BERT can obtain high performance even across languages with no lexical overlap, suggesting that the multilingual representational capacity of M-BERT is deeper than simple vocabulary memorization.

Artetxe et al. [2019] carried out a different probing experiment on zero-shot cross-lingual transfer benchmarks, but with similar observations: monolingual models indeed learn some abstractions that can be generalized across languages. They showed that the multilingual representations in M-BERT do not necessarily rely on the shared vocabulary and that the joint pre-training is necessary for comparable performance to cross-lingual models.

For their probing experiment, Artetxe et al. [2019] proposed a simple methodology to transfer a pre-trained monolingual model to a new language by just learning a new embedding matrix. To this end, they first pre-train BERT on data for language L_1 , then freeze the transformer layers and continue training on monolingual data

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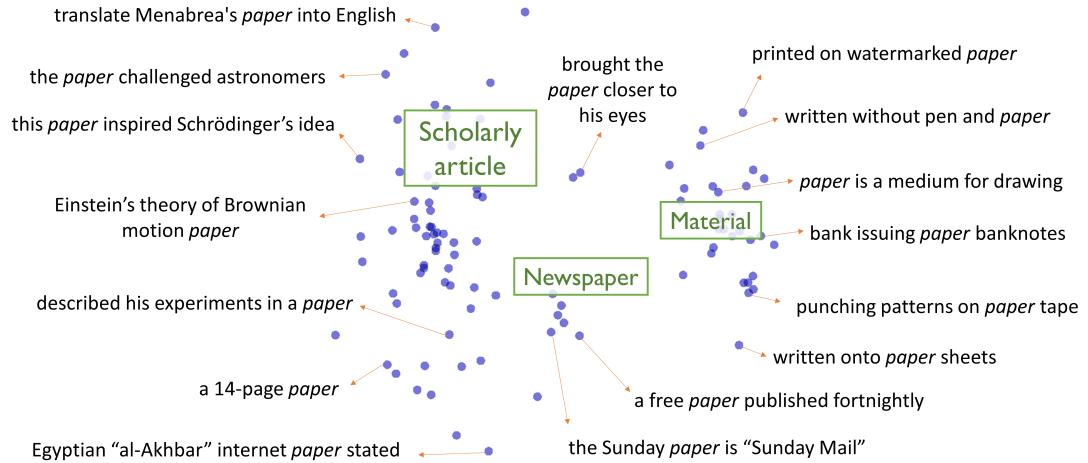


Figure 6.12: BERT contextualized embeddings for the word “paper” are clearly separated into different clusters depending on the intended meaning of the word.

from a second language L_2 in order to learn a new token embedding matrix for L_2 . The obtained model is fine-tuned on task-specific data in L_1 and then the embedding matrix of the model is swapped for the embedding matrix of L_2 . The process involves no joint training and there is no shared vocabulary given that separate subword vocabularies are used for the two languages (each learned from the corresponding monolingual data).

The importance of lexical overlap was also investigated by K et al. [2020]. The authors made a similar conclusion that lexical overlap between languages plays a negligible role in the cross-lingual success. They, however, showed that grammatical word order similarity across languages is quite important in transferability of linguistic knowledge. A similar analysis was carried out by Pires et al. [2019], suggesting that effective transfer of structural knowledge across grammatically-divergent languages would require the model to incorporate an explicit multilingual training objective, such as that used by Artetxe and Schwenk [2019] and Conneau and Lample [2019].

6.7.5 LEXICAL CONTEXTUALIZATION

Despite not having any specific objective to encourage the encoding of sense-level information, contextualized representations have proved their power in capturing deep lexical semantic information. This is highlighted by their effectiveness in various NLP tasks that require sense-specific information.

For instance, on the Word-in-Context dataset which is a test bed for evaluating the abilities of a model in capturing sense-specific information (see Section

6.7.6), BERT-based models significantly outperform classic sense representation techniques (discussed in Chapter 5). Moreover, state-of-the-art Word Sense Disambiguation models are currently powered by contextualized embeddings [Loureiro and Jorge, 2019].

To explain the effectiveness of contextualized embeddings in encoding sense-specific information, Reif et al. [2019] carried out an analysis on the semantic properties of contextualized BERT representations for ambiguous words. Figure 6.12 shows an example for the target word “paper”, with possible meanings “paper material”, “scholarly article” and “newspaper”.⁸ The three meanings are clearly separated in the dimensionality reduced semantic space.

As it is clear from the Figure, unlike classic sense embeddings, contextualized embeddings do not assign a finite number of senses to each word. Instead, the same word can be theoretically placed in an infinite number of different positions in the semantic space, depending on the context in which it appears. Ethayarajh [2019] carried out a comprehensive analysis on this property of contextualized lexical representations, specifically for ELMo, BERT, and GPT-2. They showed that it is the variety of contexts a word appears in, rather than its polysemy, that drives variation in its contextualized representations. This was highlighted by the fact that the contextualized representations for stopwords such as *the*, *of*, and *to*, which are essentially not polysemous, are among the most context-specific ones with low self-similarity across different contexts.

Another finding of Ethayarajh [2019] was that contextualized representations are anisotropic rather than isotropic.⁹ They showed that the contextualized word representations are not uniformly distributed in the semantic space (i.e., isotropic); instead, they occupy a narrow cone (i.e., anisotropic). Also, the extent of the anisotropy is magnified in the deeper layers, especially for GPT-2 in which the last layer’s representations for any two random words would be almost equal to 1.0 according to cosine similarity.

6.7.6 EVALUATION

Similarly to other types of embeddings, contextualized embeddings can be evaluated in two different contexts: *in-vitro* in which an explicit test is carried out to verify their quality, and, *in-vivo* which checks for their impact when integrated into a

⁸Illustration generated using Tensorflow’s Projector; dimensionality reduction using T-SNE.

⁹from Ethayarajh [2019]: If word representations from a particular layer were isotropic (i.e., directionally uniform), then the average cosine similarity between uniformly randomly sampled words would be 0. The closer this average is to 1, the more anisotropic the representations. The geometric interpretation of an isotropy is that the word representations all occupy a narrow cone in the vector space rather than being uniform in all directions; the greater the anisotropy, the narrower this cone.

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Label	Target	Contexts
F	bed	There's a lot of trash on the <i>bed</i> of the river I keep a glass of water next to my <i>bed</i> when I sleep
F	justify	<i>Justify</i> the margins The end <i>justifies</i> the means
F	land	The pilot managed to <i>land</i> the airplane safely The enemy <i>landed</i> several of our aircrafts
T	air	<i>Air</i> pollution Open a window and let in some <i>air</i>
T	beat	We <i>beat</i> the competition Agassi <i>beat</i> Becker in the tennis championship
T	window	The expanded <i>window</i> will give us time to catch the thieves You have a two-hour <i>window</i> of clear weather to finish working on the lawn

Table 6.1: Sample positive (T) and negative (F) pairs from the WiC dataset.

downstream NLP application. Given their desirable fine-tuning property, most evaluations have focused on the *in-vivo* setting.

An example is the GLUE benchmark [Wang et al., 2019b], which mostly focuses on sentence-level representation, with tasks such as sentence similarity, sentiment analysis, grammatical acceptability, question answering, and inference. Not long after the introduction of the benchmark, contextualized models surpassed the human level performance, leaving no headroom for further research. As an effort to making a more challenging dataset, SuperGLUE [Wang et al., 2019a] benchmark was introduced, with tasks such as multi-sentence reading comprehension, common sense reasoning, and the Winograd Schema Challenge [Levesque et al., 2012]. SuperGLUE is currently one of the widely accepted benchmarks for evaluating contextualized models.

The Word-in-Context dataset (WiC) is the only subtask in SuperGLUE that focuses on lexical semantics. A system's task on the WiC dataset is to identify the intended meaning of words. WiC is framed as a binary classification task. Each instance in WiC has a target word w , either a verb or a noun, for which two contexts are provided. Each of these contexts triggers a specific meaning of w . The task is to identify if the occurrences of w in the two contexts correspond to the same meaning or not. In fact, the dataset can also be viewed as an application of Word Sense Disambiguation in practise.

Table 6.1 shows a few sample instances from WiC. It is important to note that the task was designed to serve as a benchmark for evaluating lexical semantics. In other words, the main task is to obtain (context/sense-specific) representations for the target word and assess if these are close enough to correspond to the same meaning of the word or not. However, contextualized models are often incorrectly evaluated on the benchmark based on their effectiveness in encoding the whole sentence. Instead of taking the target word’s representation, usually, it is the sentence representations which are compared against each other to decide on the two classes.

Sentence and Document Embeddings

In the first part of the book we focus on some of the smallest units in language, mostly at the word-level. However, in most applications dealing with natural language, understanding longer units of meaning such as sentences¹ and documents is crucial.

7.1 UNSUPERVISED SENTENCE EMBEDDINGS

In this section we focus on those sentence representations that make use of unannotated text corpora as only source for building their sentence embeddings. This is similar to conventional word embeddings models (see Section 3.2), which only need for a large corpus in order to build their vector representations.

7.1.1 BAG OF WORDS

The traditional method to represent long pieces of texts has been through word-level features. Early methods in vector space models combined one-hot vector representations of words (see Section 1.3 for more details on these early methods). While this can lead to reasonable representations, their high dimensionality and sparsity has motivated researchers to explore other alternatives for combining word units. The process to represent sentences or documents through the composition of lower-level units such as words, is known as compositionality.

Compositionality. Compositionality is a key concept in language understanding. How to combine small units (e.g., words) so a longer unit (e.g., a phrase or a sentence) has been a long-studied topic in NLP. Especially after we found that we could reliably build high-quality vector representations of short units like words, as we studied in previous chapters. This naturally poses the questions on how to combine these smaller text units to accurately represent the meaning of longer

¹For a more casual survey on sentence embeddings, we would recommend the following two blog posts which have been taken as a reference for writing this section: (1) *The Current Best of Universal Word Embeddings and Sentence Embeddings* - <https://medium.com/huggingface/universal-word-sentence-embeddings-ce48ddc8fc3a> (last visited on December 2019); and (2) *On sentence representations, pt. 1: what can you fit into a single #!%&% blog post?* - <https://supernlp.github.io/2018/11/26/sentreps/> (last visited on December 2019).

units such as sentences. One of the first extensive analyses on this area is that of [Mitchell and Lapata \[2008\]](#). Different arithmetic operations such as multiplication and addition were compared, with the results pointing out to a complementarity of these operations. Later works were also inspired by linguistically-motivated vector spaces for composition. For instance, adjectives have been represented as functions that alter the meaning of nouns, which are represented as vectors [\[Baroni and Zamparelli, 2010\]](#). Similar mathematical frameworks where nouns are modelled according to other structures for verbs and adjectives have been proposed [\[Coecke and Clark, 2010, Grefenstette et al., 2011\]](#).

Approaches based on neural network have also been employed as compositional functions. For instance, recursive neural networks over parse trees [\[Socher et al., 2012\]](#) have been proved useful compositional functions in various NLP tasks such as sentiment analysis [\[Socher et al., 2013b\]](#).

More recently, a simple method based on word embedding averaging has been proved a strong alternative [\[Arora et al., 2017\]](#). This average can be weighted (e.g., tf-idf or lexical specificity) or unweighted (i.e., weights are determined by word frequency in a sentence). Postprocessing techniques such as Principal Component Analysis (PCA) are often also employed.

One of the main drawbacks of some of these compositional methods is their insensitivity to word order. This makes these methods (e.g. those based on vector averaging) unsuited to hard language understanding tasks on which word order is an essential component. For instance, sentiment analysis or language inference are tasks on which not capturing word order can be clearly detrimental. Moreover, tasks involving a generation component such as machine translation are also affected by this limitation. In the following section we present methods that aimed at learning sentence representations directly as part of the training process.

7.1.2 SENTENCE-LEVEL TRAINING

In order to overcome the lack of sensitivity of bag-of-word models to word order, direct training on sentences has been utilized for learning sentence embeddings. The main underlying idea behind these models is their capacity of predicting the surrounding sentence given an input sentence. This would provide the models understanding of isolated sentences without having to rely solely on their components (as the models presented in the previous section). In a sense, this goal is similar to standard word embedding models (see Chapter 3). For instance, in the Skip-gram model of Word2Vec [\[Mikolov et al., 2013a\]](#), given a word the goal is to predict the words in its immediate context. In this case, what is predicted is the following sentences and not words, but the underlying idea remains quite similar.

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This motivation has led to several specific models with small variations. A popular example of this kind of model is **Skip-Thought** vectors [Kiros et al., 2015]. In this model a recurrent neural network (RNN) is employed as part of a standard sequence to sequence (seq2seq) architecture, similar to that used for Machine Translation [Sutskever et al., 2014]. The training workflow of this model is as follows:

1. A sentence (e.g., “The kids were playing with a ball in the garden.”) is given as input. The goal is to predict the next sentence (e.g., “The ball fell into a flower pot.”), which we will refer to as the output sentence.
2. Using the RNN-based seq2seq architecture, the input sentence is encoded into an intermediate representation.
3. The output sentence is generated by decoding this intermediate representation.

This process is repeated for all sentence pairs in the training data, which usually sum to a large number, in the order of millions.

Alternatively, **Quick-thoughts** vectors [Logeswaran and Lee, 2018] proposed to treat the problem as classification, instead of prediction. The main difference between these two types of model are depicted in Figure 7.1. Instead of having an encoder-decoder architecture which attempts to generate the output sentence, this model will just select the output sentence from a set of sentences sampled from the reference corpus. One of the main advantages of this method is the speed, as the generation step, which is quite costly, is replaced by a faster classification procedure. This makes Quick-thoughts vectors more scalable and suitable to train on a large corpus.

Finally, it is important to highlight that recent successful sentence representations are built by relying on pre-trained language models and contextualized embeddings (cf. Chapter 6). In this case, given a pre-trained language model it is straightforward to obtain a representation of a given sentence. Reducing the complexity of pre-trained language models to obtaining an embedding per sentence has obvious advantages in similarity, clustering and retrieval tasks that would require heavy computations otherwise. Reimers and Gurevych [2019] discuss several strategies to retrieve such sentence embedding from a pre-trained language model like BERT (see Section 6.4). The most common strategies are retrieving a single contextualized embeddings as sentence embedding, or performing an average between all contextualized embeddings of the sentence.

7.2 SUPERVISED SENTENCE EMBEDDINGS

This branch of sentence embeddings make use of additional resources in addition to unlabelled text corpora. Training on unlabeled corpora can be limiting and these

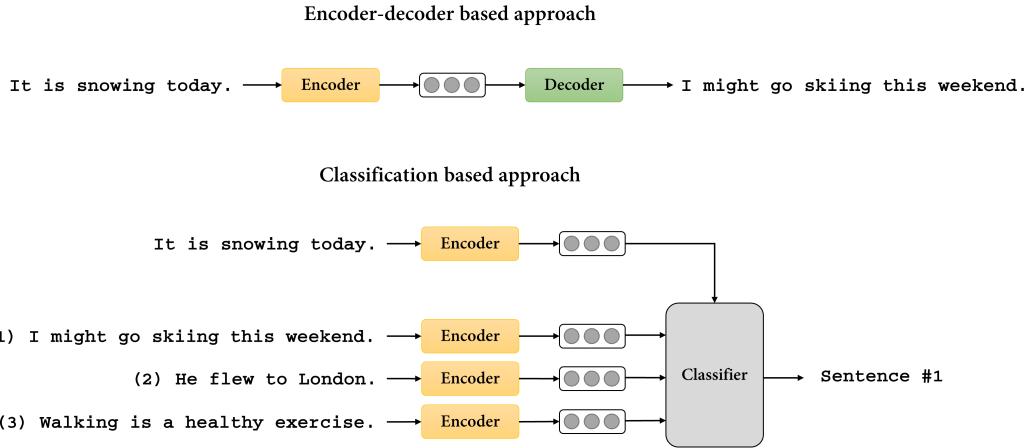


Figure 7.1: High-level overview of unsupervised sentence embedding techniques. On the top an approach based on generation and at the bottom an approach based on classification.

approaches exploit diverse sources aiming at improving the quality of unsupervised representations.

1. **Language Inference data.** Language inference is a task to determine whether a statement entails, contradicts or is neutral with respect to a premise. It has often been considered an important proxy to language understanding. This task has also been known as textual entailment and since recent years large-scale benchmarks such as SNLI [Bowman et al., 2015] or MultiNLI [Williams et al., 2018] have been developed. In the context of sentence embeddings, Conneau et al. [2017] developed a bidirectional LSTM encoder that takes the sentence pairs from the SNLI corpus as external supervision.
2. **Machine Translation.** An external task that has been used to learn sentence embeddings is neural machine translation. The signal that translations of different sentences provide is complementary to unsupervised methods of training sentence representations from an unlabeled corpus. For instance, McCann et al. [2017] incorporates a network that updates the weights of sentence embeddings during training, which are then combined with their CoVe contextualized word representations (cf. Chapter 6).
3. **Vision.** In some cases, language comes together with different modalities, such as acoustic or visual features. For instance, images are frequently accompanied with captions, which encourages the development of system which takes ad-

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vantage of both modalities for language understanding. [Kiela et al. \[2018\]](#) proposed a sentence embedding model that aims at predicting visual features from the image associated with the caption (sentence). In this case the sentences are encoded with a bidirectional LSTM which are then enriched with the visual features prediction.

Multitask learning. In general, all these different aspects of the same sentence can be encoded into a multitask learning framework. Multitask learning in NLP has been popularized since the early work of [Collobert and Weston \[2008\]](#). While it has been shown to have potential to improve NLP tasks by leveraging similar tasks where data is available [[Peng et al., 2017](#), [Ruder, 2017](#)], its current utility for certain settings has also been discussed [Bingel and Søgaard \[2017\]](#). In the context of sentence embeddings, [Subramanian et al. \[2018\]](#) leveraged several NLP tasks (including language inference and machine translation) into a unified multitask learning framework to learn general purpose sentence representations. Similarly, [Cer et al. \[2018\]](#) encode sentence into a transformer-based architecture that includes a variety of language understanding tasks.

7.3 DOCUMENT EMBEDDINGS

In this section we explain specific approaches to model units longer than sentences, in particular documents². While some of the approaches mentioned in the previous sections can also be used to model documents, representing documents usually need lighter models (approaches based on neural networks can be quite expensive to represent documents). Because of this, bag of word models tend to be popular to learn representations of these longer units of text such as documents. As with sentence embedding bag-of-word techniques (cf. Section 7.1.1), these approaches are often sub-optimal as word order is not taken into account. However, this limitation is less pronounced for documents as context is larger.

A popular technique to induce topics from documents, which can then be used as a document representations, are based on Latent Dirichlet Allocation [[Blei et al., 2003b](#), **LDA**]. This method is based on generative probabilistic model that employs a hierarchical Bayesian structure to infer the latent topics within text corpora. More recently, and similarly to word embeddings techniques such as Word2Vec (cf. Chapter 3), approaches going beyond count-based bag of word methods often involve some kind of predictive behaviour. [Le and Mikolov \[2014\]](#) proposed a language model-based architecture to predict the words occurring in a given document (or paragraph).

²Some approaches also model paragraphs but in the main the distinction is not made, and approaches for either unit (paragraph or document) can be applied interchangeably.

[Kusner et al. \[2015\]](#) also showed that relying on the word embeddings of a given document is in most cases enough to be able to infer a reliable semantic similarity metric among documents.

7.4 APPLICATION AND EVALUATION

One of the main advantages of encoding portions of texts into fixed-length vectors is its flexibility. Sentence and document embeddings can be applied to any tasks involving these linguistic units, with the added benefit of being computationally cheaper than other methods involving supervised classifiers such as neural networks. In particular, they are particularly attractive for applications involving large amounts of computation such as information retrieval or clustering of documents.

Sentence level. The spectrum of application for sentence level tasks is immense. As mentioned earlier, many NLP tasks involved some kind of sentence processing in one way or another. Tasks such as sentiment analysis or language inference, to name but a few, can often be framed as sentence classification. In order to provide a unified framework with different tasks, two efforts have been presented. First, SentEval [[Conneau and Kiela, 2018](#)] contains a variety of sentence-level tasks including sentiment analysis, sentence similarity, language inference and image caption retrieval. As part of the framework supervised classifiers are provided so as to compare the underlying sentence representations directly. Second, the language understanding benchmarks GLUE [[Wang et al., 2019b](#)] and SuperGLUE [[Wang et al., 2019a](#)] are mostly composed of sentence-level tasks (cf. Section 6.7), and hence are suitable to test and apply sentence embeddings on. Finally, semantic and syntactic probing tasks have also been proposed as a way to have a more linguistically-grounded evaluation of sentence embedding techniques [[Conneau et al., 2018a](#)]. [Perone et al. \[2018\]](#) provide an extensive empirical comparison involving both downstream and linguistic probing tasks.

Document level. The evaluation at the document level has been almost exclusively focused on text categorization. In text categorization various categories are pre-defined and the task consists of associating a given input document with the most appropriate category. This task is often framed as supervised classification, where documents with their gold categories as given as training data. The most usual domain for the evaluation is newswire [[Lewis et al., 2004](#), [Lang, 1995](#), [Greene and Cunningham, 2006](#)], while text categorization datasets for specialized domains are also available, e.g. Ohsumed [[Hersh et al., 1994](#)] - medical.

CHAPTER 8

Ethics and Bias

Most current Machine Learning models are data-driven: they learn from the data to which they are exposed. Therefore, it is an inevitable consequence that they inherit all the implicit gender, racial, or ideological biases from the data, unless some measures are taken into account to prevent this. Addressing harmful biases is crucial because machine learning models have now passed the “experimental” stage and have directly entered people’s lives in different areas, such as criminal justice, online advertising, and medical testing, where they can have various implications.

An example is a study by MIT Media Lab on gender and skin type performance disparities in commercial facial recognition models [Raji and Buolamwini, 2019]. Initial results of this study revealed a strong bias against women and darker skins in gender classification and resulted in a sequence of updates to these models for addressing the bias. Another example is the study of a risk assessment tool that was widely used in criminal justice, carried out by ProPublica. The tool used to predict the probability of a defendant to commit a crime in the future. The study found that risk estimates had a strong bias against African-American defendants.¹

In fact, during the past few years, with the wide-spread use of data hungry deep learning models, the ethical aspect in predictive models has raised as important concern which is worthy of more attention and investigation [Zhao et al., 2017]. Public sensitivity to this topic is very much highlighted by the wide objection over the “emotional contagion” experiment of Facebook [Kramer et al., 2014].

NLP models are usually trained on text corpora as their main source of knowledge; hence, they are prone to learning all the inherent stereotyped biases that reflect everyday human culture. In a nominal study, Caliskan et al. [2017] showed that text corpora usually contain imprints of our historic biases, whether “morally neutral as toward insects or flowers, problematic as toward race or gender, or even simply veridical, reflecting the status quo distribution of gender with respect to careers or first names”.

Bender and Friedman [2018] highlight the importance of having knowledge about characterization of a dataset we use for training a model, which would allow us to better understand the potential biases reflected in the model and to have an idea on the extent to which the results may generalize to other domains. They propose a

¹<https://www.propublica.org/article/machine-bias-risk-assessments-in-criminal-sentencing>

he	maestro, skipper, protege, philosopher, captain, architect, financier, warrior, broadcaster, magician
she	homemaker, nurse, receptionist, librarian, socialite, hairdresser, nanny, bookkeeper, stylist, housekeeper

Table 8.1: The closest occupations to the embeddings of words *she* and *he* in the embedding space of Word2vec Google News. Results by [Bolukbasi et al. \[2016\]](#).

“data statement” schema which involves various type of information, such as source of texts used, language variety, and annotator demographic.

[Hovy and Spruit \[2016\]](#) overviewed the social impact of NLP research and highlighted various implications of bias in NLP, including (1) demograpgic mirepresentation and **exclusion** of the language used by minority groups making the technology less suitable for them, hence reinforcing the demographic differences; (2) **Overgeneralization** which is a modeling side-effect and a consequence of negligence over false positives; and (3) topic **overexposure**, which is particularly relevant for the choice of languages under research which is mostly centered around a few languages only, directly impacting typological variety.

8.1 BIAS IN WORD EMBEDDINGS

Given what was described above, it is natural for word embeddings to encode implicit bias in human-generated text. In a seminal work, [Bolukbasi et al. \[2016\]](#) studied the existence of gender bias in word embeddings. The results pinpointed female/male gender stereotypes to a disturbing extent. This was surprising as the studied word embeddings were the standard Word2vec embeddings trained on Google News articles which are written by professional journalists.

[Bolukbasi et al. \[2016\]](#) extracted the closest occupations in the word embedding space (Google News Word2vec²) to the words *he* and *she*. The results are shown in Table 8.1. The list was evaluated by crowdworkers and was identified to have strong indications of gender stereotypicality. [Bolukbasi et al. \[2016\]](#) observed similar unwanted gender biases in an analogy test. They extracted from the embedding space the set of analogous word pairs to *he-she* with the condition that the pair are semantically similar to each other. Many of the identified pairs were classified by crowdworkers to exhibit gender stereotypes. Sample pairs are shown in Table 8.2.

8.2 DEBIASING WORD EMBEDDINGS

This existence of gender-specific stereotypes in word embeddings is particularly important not only because they reflect gender bias implicit in text but also, given their

²Similar results were observed using GloVe web crawl embeddings.

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gender stereotype analogies	gender appropriate analogies
sewing-carpentry, registered nurse-physician, housewife-shopkeeper, nurse-surgeon interior designer-architect, softball-baseball, blond-burly, feminism-conservatism, cosmetics-pharmaceuticals, giggle-chuckle, vocalist-guitarist, petite-lanky sassy-snappy, diva-superstar, charming-affable, volleyball-football, cupcakes-pizzas lovely-brilliant	queen-king, sister-brother, mother-father, waitress-waiter, ovarian cancer-prostate cancer, convent-monastery

Table 8.2: Analogous pairs to *he-she* generated by [Bolukbasi et al. \[2016\]](#).

widespread use, these embeddings can potentially amplify the bias in the society. Therefore, it is crucial to seek techniques for reducing or discarding bias from word embeddings. Recently, there has been efforts to mitigate gender bias in word embeddings either as a post-processing stage [[Bolukbasi et al., 2016](#)] or as part of the training procedure [[Zhao et al., 2018](#), [Lemoine et al., 2018](#)]. [Sun et al. \[2019\]](#) provide a review of the literature on mitigating gender bias in NLP. One of the first attempts at debiasing word embeddings was carried out by [Bolukbasi et al. \[2016\]](#). The authors quantified bias for a word w based on its relative distance to pairs of gender specific words (such as *brother*, *sister*, *actress*, and *actor*). The word w is said to possess gender bias, if the distances of w to the gender specific words in pairs are unequal. In other words, to compute gender bias for w , they projected the embedding of w to “the gender direction”. The value of this projection was taken as the extent of bias for w . The gender direction is computed by combining³ the differences of ten gender-specific terms, such as *she* and *he*, *her* and *his*, and *woman* and *man*.

[Bolukbasi et al. \[2016\]](#) used a post-processing technique for debiasing word embeddings. For each word in a word embeddings space, they neutralize the gender projection on the “gender direction”. They also make sure that all these words are equi-distant from the predefined gender-specific pairs. [Lemoine et al. \[2018\]](#) used the gender direction of [Bolukbasi et al. \[2016\]](#) and learns a transformation from the biased embedding space to a debiased one using adversarial training. [Zhao et al. \[2018\]](#) took a different approach and propose training debiased embeddings by changing the loss function in GloVe model. The change is targeted at concentrating all the gender-specific information to a specific dimension which they can discard to produce gender-debiased word embeddings.

The above works differ in their methodology but all share a similar definition of bias: being neutral with respect to the gender direction. However, [Gonen and Gold-](#)

³More specifically, gender direction is computed as the principal component of then ten gender pair difference vectors.

berg [2019] showed through a set of experiments that this definition is insufficient for determining bias and the bias reflecting world stereotypes is much more subtle in the embeddings. Specifically, they observed that there exist a systematic bias in the embeddings which is independent of the gender direction and removing this “remaining” bias requires scrutinizing embeddings at much deeper levels.

Conclusions

In this book, we aimed at providing a high-level introduction to various embeddings used in Natural Language Processing. To this end, we covered early works in word embeddings and more recent contextualized embeddings based on large pre-trained language models. The currently celebrated contextualized embeddings are the product of a long path of evolution. Since the start, distributional hypothesis has been the dominating basis for the field of semantic representation and prevailed even for recent models; but, the way of constructing representations has gone under a lot of change. The initial stage of this path is characterized by models that explicitly collected co-occurrence statistics, which often needed a dimensionality reduction (Chapter 3). Together with the revival of neural networks and deep learning, semantic representation experienced a massive boost. Neural networks provided an efficient way of processing large amounts of texts and directly computing dense compact representations. Since then, the term “representation” was almost fully substituted with their dense version, called “embeddings”. This development path has revolutionized other fields of research such as graph embeddings (Chapter 4) or resulted in the emergence of other fields of research, such as sense embeddings (Chapter 5), and sentence embedding (Chapter 7).

A recurring trend to note is the rapid pace of development in the field of semantic representation. For instance, upon its introduction in early 2018, ELMo (Chapter 6) occupied the top of most NLP benchmarks. However, in just less than a year, BERT significantly outperformed all previous (feature extraction-based) models, including ELMo. The development has not stopped though with several new contextualized models giving further boosts. These models currently approach (or even pass) human-level performance in many of the standard NLP benchmarks, such as SuperGLUE [Wang et al. \[2019a\]](#). However, it is clear that in many fields, such as question answering with common sense reasoning, machine translation, and summarization, there is a big room for the improvement of NLP models. In other words, the “true” natural language understanding is far from reached. This shows certain biases towards these datasets, which is inevitable, and highlights the need for the introduction of new datasets or benchmarks for more rigorous evaluation of our models and for measuring our progress towards concrete goals.

Another point of concern is that NLP research has mostly focused on the English language and for settings in which abundant data is available. Extending this tools/knowledge to languages other than English, especially resource-poor languages, and to other domains for which little data is available, is another problem which is open for research. Also, almost all these techniques are purely text-based. Incorporating semi-structured knowledge, such as knowledge encoded in lexical resources or semantic/syntactic priors of a given language remains as another research challenge. It is also noteworthy to mention that due to the deep learning hype, the current research in NLP is getting dismissive of the importance of linguistic aspects, ignoring the decades of methodological and linguistic insights. This is also relevant to semantics, which is the main topic of this book. It is necessary to step back and rethink, which should probably be inevitable for true language understanding.

Last but not least, deep learning models are known to be blackboxes. It is difficult to ask models or to investigate the reason behind their decisions. With respect to semantic representation, embeddings are generally not interpretable. Another area of research can investigate the problem of explaining these representations and what they (do not) capture, in the line of [Hewitt and Manning \[2019\]](#).

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